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Enhancing Learning with Online Resources, Social Networking, and Digital Libraries

EDITED BY
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and Harry E. Pence

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Before agreeing to publish a book, the proposed table of contents is reviewed for appropriate and comprehensive coverage and for interest to the audience. Some papers may be excluded to better focus the book; others may be added to provide comprehensiveness. When appropriate, overview or introductory chapters are added. Drafts of chapters are peer-reviewed prior to final acceptance or rejection, and manuscripts are prepared in camera-ready format.

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Dedication

We thank our wives, Waree S. Belford, Elizabeth A. Moore, and Virginia W. Pence, for their patience and help in bringing this volume to fruition.

We express our appreciation to the staff of ACS books who have provided so much support and advice to us.

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Chapter 1

An Introduction to Enhancing Learning with Online Resources, Social Networking, and Digital Libraries

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Our science and our society are in the midst of a digital revolution that is changing the way that we use information, communicate and share information with others, and participate in social groups to address problems. How will education in general and chemical education in particular respond to these dramatic changes? Early adopters are exploring a broad range of possibilities. This book is the first volume of a series of books which we envision to showcase the current state of the art based upon material presented in symposia at ACS national meetings, BCCEs, Online ConfChem conferences and other venue. It will be of interest to anyone who wants to enhance learning and involve students with the panoply of evolving information and communication tools that are available for scientific research and education.

The World Wide Web has had a profound impact on scholarly communication and the dissemination of resources. Preparing students for this new environment will require significant changes in the educational process. At the same time, new kinds of computer software are making it much easier to create groups of people with similar interests. New tools, like RSS feeds, and social tagging are changing the way that

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readers interact with information. Wikipedia, where articles are written and edited collaboratively by volunteers from around the world, has become a model for many similar efforts. This type of crowdsourcing opens up new avenues for information processing, research, and collaborative learning. Some argue that these successes are a prelude to a more general movement toward openness in the scholarly process.

This book addresses these questions and their implications:

- How are cheminformatics and the digital revolution changing students' ability to acquire information, and how can instructors take advantage of this to enhance learning?
- What learning opportunities arise as students deal with assessing the veracity of information acquired through disparate resources?
- What are suitable sustainability models for content development in the new open access, open source, open data, open publishing world?
- How do digital libraries support development of new resources, collections of resources, maintenance of resources, and communication among teachers and students?
- What new types of educational resources have been developed by open-source projects and what new opportunities do they offer educators?
- How can social networks, social tagging, wikis, and other tools best support and contribute to students' learning?
- How are these new tools and attitudes affecting the traditional process of scholarly communication?

Several years ago, Carla Hesse, a prize-winning historian from UC Berkeley, wrote about her vision of the future of scholarship (Hess, C. Books in Time. In *The Future of the Book*; Nunberg, G., Ed.; University of California Press: Berkeley, CA, 1996; p 31.), "In the future, it seems, there will be no fixed canons of texts and no epistemological boundaries between disciplines, only paths of inquiry, modes of integration, and moments of encounter." If her prediction is correct, and it seems to be coming true, this will have a major impact on all aspects of teaching and learning, including chemical education. It is important that educators, students, and the public become aware of the implications of online resources, social networking, and digital libraries for scientific education and research. Many opportunities are ripe to be seized and the contributors to this

> book are at the forefront of determining which are most useful and effective.

Information and Communication Technologies (ICTs) are changing the way our society stores and communicates information. This ACS Symposium Series Book is a collection of papers that highlight various impacts these changes have had—and can have—on the chemical education community. In the chapters of this book we have brought together papers that cover a broad range of topics. These include generalized topics on information management, Open Science, Open Resources and the digital revolution, along with descriptions of specific resources such as the RSC ChemSpider, the Organic Reaction Explorer and various collections of the Chemical Education Digital Library. There are contributions on Open Source software development in the chemical sciences and the application of chemical education research to the development of animations and online learning environments. It is our intention that the collection of papers presented in this book will provide information that will be useful to traditional academicians, their students, and free agent learners who seek to take advantage of online resources in the pursuit of teaching and learning.

Although this ACS Symposium Series Book is sponsored by the ACS Division of Chemical Education (DivCHED) (*1*), we recognize that ICTs impact scholarly communication in many disciplines. Thus we have included papers from non-chemistry sources as well as papers based on presentations at ACS National Meetings, Biennial Conferences on Chemical Education (*2*), online ConfChem (*3*) conferences, and the ChemEd DL (*4*). Although we have focused on chemical education, we hope that this book will be of use to anyone in who is interested in how ICTs can enhance learning, not only in formal and informal environments, but also with respect to scholarly activities in education and research.

Two challenges in putting this book together were that we were using a traditional book to describe the rapidly changing concept of what a book *is*, and that a single book cannot adequately cover such a broad topic. Web 2.0 digital technologies such as wikis are creating dynamic, perpetually evolving, multi-authored texts that blur the distinction between readers and authors. Simply put, there is an inherent error in thinking that a static, hard-copy book can faithfully represent how Web 2.0 technologies have changed our conception of a book. With respect to the second challenge, we expect that this volume will be the first of a series of ACS Symposium Series Books on this subject, each representing a snapshot in time of this important field. We do not claim that any single book can be a comprehensive treatise on the subject, but we hope that this collection will be of value to both experts and novices who are trying to understand and take advantage of the evolving nature of education and scholarly communication in the chemical sciences.

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Part I: Online Resources: Open Science and Open Resources

Users of online resources are faced with two major questions: To what extent can I rely on what I am reading? and, How can I use it?—or *Can* I use it? The open nature of the World Wide Web has led to proliferation of both accurate and inaccurate information; in addition, a plethora of different approaches to copyright has been disseminated and repurposed by both novices and experts in appropriate and inappropriate ways. Thus a logical starting point is to look at the open nature of the Web and see what impact this has on education and on science in general. Even a concept like "Open Access" can have multiple interpretations, as John Willinsky points out in "Ten Flavors of Open Access to Journal Articles" in Appendix 1 of his book "The Access Principle: The Case for Open Access to Research and Scholarship." (*5*) These flavors range from instant free access to material along with permission to create derivative works (the Budapest Open Access Initiative (*6*) definition), to delayed or partial open access with restricted usage (only subscribers get instant or complete access). All forms of open access involve access to material on the Web without paying a fee, but educators' need to repurpose material leads to the concept of "Open Resources", those that are open access in the Budapest Initiative sense, with copyright licenses like General Public License (GPL) (*7*) or Creative Commons (*8*) that allow for repurposing and production of derivative works. Two Open Resource sites of interest to educators are the United Nations Educational, Scientific and Cultural Organization Open Educational Resource (*9*) and SchoolForge.net (*10*).

Chemical educators need to understand the impact of the open nature of online resources on both science and education. The concept of Open Science is a latent theme of several chapters in this book. A very important Open-Science community in chemistry is Blue Obelisk (*11*), a group of chemists, programmers and chemical informatics professionals who promote Open Science through the "three pillars of the Blue Obelisk movement": Open Data, Open Standards and Open Source (ODOSOS) (*11*). All authors in this first section of the book have been involved with Blue Obelisk.

Open-Science movements such as Blue Obelisk are far more important to chemical educators than simply the Open Resources they are creating. The movement is changing the way science is performed. Consider the four goals of Open Science as defined by Dan Gezelter in his OpenScience.org blog (*12*) essay: "What, exactly, is Open Science" (*13*)

- Transparency in experimental methodology, observation, and collection of data.
- Public availability and reusability of scientific data.
- Public accessibility and transparency of scientific communication.
- Using Web-based tools to facilitate scientific collaboration.

This first section looks at several ways the Open Science movement is changing the way we do science and potential implications for chemical education.

Part of the problem with reliability of the Web as a source of information stems from the fact that today's search engines are not designed to assist the

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user in critically evaluating the information delivered. There is a clear need for online services that can assist users in evaluating the accuracy of the chemical information they access and acquire. A new resource in this area is the Royal Society of Chemistry's ChemSpider, a portal to online chemical information and resources. Antony Williams, one of the developers of ChemSpider, has provided a chapter, "ChemSpider: Integrating Structure-Based Resources Distributed across the Internet", that describes it. ChemSpider not only aggregates data and links to both open and proprietary databases, but also includes a reviewed, crowd-sourced curation of data based on a hierarchical structure that helps users assess the data's accuracy. The site allows for a variety of flexible search approaches including structure and substructure queries of a chemical data base containing almost 25 million unique chemical compounds.

ChemSpider was not originally designed as an educational tool, but its developers understand the importance of chemical education and have provided interfaces that enable development of tools of value to educators. One such tool is the Spectral Game (*14*), in which students competitively associate spectra with structures. (Interestingly, the game can also be used in the curation process of published data.) Another tool, ChemSpider Synthetic Pages (CS/SP) (*15*), is a peer-reviewed online publishing platform for chemical synthesis reactions and procedures; it enables students to publish reactions without submitting a formal publication. Synthetic Pages also utilizes social networking functions by which authors can receive feedback on their work, thereby enhancing learning and helping students develop online reputations and collaborations.

As educators, we need to realize that Wikis, Blogs, Podcasts, Social Networks and other Web 2.0 components not only afford us with new opportunities for enhancing learning, but also enhance our ability to communicate and perform research. One of the big questions for the future is: How will Web 3.0 technologies and the Semantic Web impact both education and scientific research? In "Using Semantically-Enabled Components for Social-Web Based Scientific Collaborations", Omer Casher and Henry Rzepa provide an overview of the use of Web 2.0 and Web 3.0 technologies, including a discussion of how these components can advance research by enabling scientific communication both within and across disciplines. Web 2.0 technologies foster collaborations by enabling interactive sharing of information over the Web while Web 3.0 technologies enable sharing of information through software agents. The authors emphasize that such technologies are complementary, not competitive.

Casher and Rzepa introduce the concept of the Semantic Web and current technologies that could enhance collaborative scientific research in a culture of Open Science. This chapter will give chemical educators a better understanding of the potential impact of the Semantic Web on how science is performed and of the technologies that are currently available. If ICTs are enabling Open Science, then it is imperative that chemical educators understand the evolution toward Open Science.

Clearly ICTs have had a huge impact on software development. Through Web 2.0-enabled communities that have sprung up in association with Sourceforge (*16*), Github (*17*), Cpan (*18*) and similar collaborative environments, programmers are now able to share code and expertise in the spirit of collaboration based on a common interest in a specific project without ever having to meet face-to-face. These communities have given educators with programming skills the opportunity to develop highly productive collaborations that have created educational applications that simply would not have yielded the financial return necessary for commercial investment. In effect, this has changed the driving force for software development from a corporate profit motive to the very practical needs of a widely dispersed community of educators.

One open-source effort that is ubiquitous in chemistry is the Jmol molecular visualization project. “Web-Based Molecular Visualization for Chemistry in the 21st Century” by Bob Hanson, at present the principal developer of Jmol, gives us a feel for the current state of Jmol. It also provides insight into the evolution of open-source applications like Jmol and how development of such a resource can be driven by input from an involved user community. Through ODOSOS, Jmol has become much more than a molecular viewer: it is effectively a Semantic Web software application that, by interacting with other software applications, can both deliver chemical structures from key Web resources and create them itself.

An example of Jmol’s versatility is its integration into the ChemEd DL WikiHyperGlossary (WHG) project. WHG is a glossary-generating program that automates the markup of digital text documents and Web pages. If a glossary term in the WHG is a chemical name, that name can be associated with an open-standard IUPAC InChI (*19*) chemical identifier. The identifier can be used to search the Models 360 (*20*) database of ChemEd DL; if the molecule is present in Models 360, clicking on its link will pop up a Jmol display to show electrostatic potentials, molecular vibrations (along with links to associated IR spectra), symmetry elements, or molecular orbitals. If the molecule is not part of the Models 360 database, a model is generated on the fly by passing the chemical identifier to other software agents. Thus a reader can submit to the WikiHyperGlossary a digital text document (MS Word, Adobe PDF…) or Web page containing the name of a compound and have nearly instant access to that compound’s three-dimensional structure, spectra, and other associated information. This has been made possible by ODOSOS.

The last chapter of this section looks at Wikipedia, which has become an important online source of chemical information. A significant fraction of faculty and students question the reliability of Wikipedia. For example, in 2009 and 2010, general chemistry students at the University of Arkansas at Little Rock were asked: “Do you use Wikipedia?” and “Do you consider Wikipedia to be a valid source of information?” The most common response to the first question was yes; however many of the students who responded positively to the first question responded no to the second. Responses such as, “No, because my teachers tell me I cannot trust Wikipedia” were common. This contradiction indicates inadequate understanding of Wikipedia’s chemistry content by many educators. Martin Walker’s chapter, “Wikipedia as a Resource for Chemistry”, should help students and educators better understand this valuable resource. Better understanding should lead to more effective use of Wikipedia.

Walker points out that understanding what Wikipedia is *not* is fundamental to understanding what it *is*. Wikipedia is neither a textbook nor a place to publish opinion or original thought; every contribution should have references

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and citations to the original source. Emphasis on verifiable information is critical to doing good science, so Wikipedia provides a microcosm akin to scientific communication. That is, understanding how to ascertain the appropriateness and verifiability of information is an important skill no matter what the information source, and we do not want our students to uncritically believe anything they read. We want them to question what is written and to learn how to dig deeper and evaluate the source of information before using it.

Walker describes several specific chemistry-related Wikipedia features, such as the "Chembox", and discusses ongoing efforts and issues associated with curating Wikipedia's chemistry content. He also points out that Wikipedia and WikiCommons (*21*) are a good source of images, graphs and charts. This leads to a discussion of the importance of teaching students how to use online material properly with respect to copyright when they incorporate it into their own classroom projects such as papers and PowerPoint presentations.

The chapters in this first section are intended to provide better understanding of specific online resources and enhanced appreciation of the importance of Open Science and Open Resources in chemical education and in the pursuit of science

Part II: Social Networking and Chemical Education

Over a decade ago, Clayton Christensen described the difference between sustaining and disruptive technologies (*22*). Sustaining technologies improve current practices in a company or organization without requiring major alterations in the way that things have always been done; disruptive technologies require dramatically different ways of operating. Christensen noted that well-established, successful companies often resist major changes in their business models and may be forced into bankruptcy by new competitors who are willing to embrace disruptive technologies. To date, professors and administrators appear to have been more willing to accept sustaining technologies, like PowerPoint and clickers, than to adopt practices that disrupt traditional methods of teaching.

Information is so fundamental to the chemical enterprise that significant changes in the way it is organized, used, and stored are very likely to be disruptive. This section of the book describes ongoing revolutions in information technology and suggests ways in which higher education might respond. The term "digital divide" has historically referred to a division between those who have or do not have computers. A more dangerous separation may well be that some people will not have the training and experience needed to use computers in more sophisticated and more powerful ways. This divide will depend upon appropriate training in the use of new technologies as well as access to online information sources.

Many colleges subscribe to at least a basic online set of American Chemical Society journals, but students at some smaller colleges may not have online access to the scientific literature they need to become proficient at modern information management. Even institutions that do have access may not all teach the skills that enable their students to become effective chemists. The papers in this section attempt to provide a better understanding of potentially disruptive information

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technologies and to answer the question, "What kinds of skills should current undergraduates learn?"

In “Sceptical Chymists Online”, Burke Scott Williams provides a historical perspective on changes that are occurring in science and science education. He suggests that much of science continues to be based on the assumptions of the Gutenberg era even though the Internet has begun to change the existing structure. Williams contends that, based on the time that it took for the printing press to change society, this may be a slow revolution—one that will take place over the coming century. Since the 17th Century, science and science education have shifted from the *Village* mode, small groups with strong personal ties to each other, towards a structure that is best described as a mixture of the *Cathedral* and the *Bazaar*. Decision making in the *Cathedral* mode is strongly hierarchical, whereas it is diffuse and informal in the *Bazaar* mode. Williams suggests that the Internet is pushing society more strongly towards the *Bazaar* mode.

Williams observes that the Scientific Revolution was brought about by improved communication (the printing press), combined with Bacon’s experimental method. While there have been many changes in communications since the 17th Century, the social aspects of science have remained relatively small (the research group, the small, intimate conference). In Christiansen’s terms, changes have been sustaining for a long time. The Internet now can support *huge* social networks of scientists—networks that are more conducive to the *Bazaar* than the *Cathedral*. Despite this, science teaching continues to follow a *Cathedral*-like, highly institutionalized organizational pattern. As science invariably moves towards a more open organization structure, it is essential that the educational process keep pace, even though the changes required may well be disruptive.

In “Creating and Using a Personalized Information Management System”, Pence and Pence argue that the proliferation of online information sources has made information overload an increasingly critical problem—one that must be addressed in undergraduate chemical education. They suggest that powerful new tools be introduced at the undergraduate level so that future chemists can work more effectively in the modern networked environment; examples are microblogging, social tagging, and Really Simple Syndication (RSS). Microblogging sites, such as Twitter, allow an individual to create a network of people with similar interests who collectively search for and share new information. Really Simple Syndication automates the search process, delivering the latest news from a variety of sources to a single, personal Web page. Social tagging, such as Delicious, Diigo, or Connotea, helps an individual organize information after it has been located and identified. Google Jockey is somewhat different, since it is designed to introduce a visual component into seminars and other classroom activities where normal methods for introducing images are not effective.

Pence and Pence describe specific examples of successfully integrating such technologies into their classrooms. Each technique might well be classed as sustaining, but the overall impact of all these changes seems more likely to be disruptive. The authors argue that, although a few students may have encountered these Web technologies outside the chemistry classroom, most lack the comprehensive understanding that results from systematic training applied to situations that chemists encounter in their professional careers.

Losoff and Pence, in “Preparing for the New Information Paradigm”, argue that chemical education should reflect changes in the way chemical research is being done. Online journals are altering access to information: more rapid distribution of articles; easier access to supporting material; faster and more comprehensive searches; and inclusion of full-color graphics, video clips, and animations. Even more disruptive developments are probably ahead. Digital technologies, especially online scholarly journals and eBooks, are linking articles, databases, and people in new ways that produce new patterns of literature use. The World Wide Web connects more than Web pages: it connects people who are building extended scholarly research networks. A loosely organized movement is calling for "open chemistry". This process is still in the early stages but will probably accelerate in the future to create more sophisticated methods for connecting. Portable devices like iPads and smartphones will contribute to a mix that will make all information available from any location, creating a virtual information commons.

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Part III: Online Resources: Pedagogy and Curriculum

Chapters in the first two sections of this book demonstrate many facets of the new milieu created by information and communication technologies. The last two sections shift the focus to a more practical vein: how ICTs can actually enhance learning. How is the role of the textbook evolving? What guiding principles do learning theories provide for developing online activities and animations? How are early adopters integrating these technologies into their curricula? While it is impossible to represent every facet of this expanding field, we hope that these chapters will be useful to those who want to use ICTs in their classrooms.

The digital revolution’s impact on the publishing industry, both within and outside academia, is a theme common to many chapters in this volume. The textbook is *the* repository of information in traditional academic curricula, so one could ask, do students really value textbooks? The flourishing used-textbook industry is one indication that they do not—except in the specific course for which the book was designed. Unpublished data from Shorb and Moore, authors of a chapter in Part IV, indicates that only about two thirds of students use their textbook extensively even in the course for which it was designed. Although students spend a lot of money for textbooks, they apparently do not consider textbooks to have long-term value. When the textbook goes online, it becomes much more adaptable to a student’s needs and interests. One can envision a future “chemistry eBook” where a student has a single “book” containing the textbooks of all classes from first year to graduation and also containing the student’s personal notes, annotations, problem-solving efforts, links to other sources, and more.

David Lubliner has outlined the evolution of eBooks in his chapter, “Integrated Learning Environments: From eBooks to e^{2}Books; From e-Learning 3.0 to e-Knowledge and Beyond”. Lubliner defines an eBook as a static *"electronic counterpart of a printed book"* that can be viewed through electronic devices, and an e^{2}Book as a dynamic eBook that uses semantic terminology to link concepts with both internal and external data sources and knowledge repositories. This can result in an Integrated Learning Environment (ILE) which Lubliner defines as an "*evolutionary environment that links dynamic books, knowledge repositories and provides organic growth to ensure the relevancy of the learning environment"*. He presents results from the implementation of an ILE, the Constructivist Unifying Baccalaureate Epistemology (CUBE), in the computer sciences program at the New Jersey Institute of Technology (NJIT). Students who utilized the CUBE for two years received 25% higher mean scores on a content examination than students who did not utilize the CUBE ILE.

Although the work at NJIT was in computer sciences, chemical educators will find much of interest in their experiences. Are textbooks evolving towards configurable e^{2}Books where students' eBook readers not only keep all of the information of an entire degree program at their finger tips, but also connect the topics of upper level courses back to their foundation courses? Such "degree level books" would span different disciplines. If a student in physical chemistry needed help with calculus an e^{2}Book could direct the student to the "text" the student used in calculus. Likewise, a person studying an upper level biology course could be seamlessly connected with the foundation chemistry material. It would all be in the student's degree level e^{2}Textbook.

Digital technologies also enable external visualizations in the form of animations and simulations that novices can use to develop understanding. It is important that educators be aware of what research has shown about developing learning activities based on these technologies. Roberto Gregorius's chapter, "Good Animation: Pedagogy and Learning Theory in the Design and Use of Multimedia", provides an overview of this important aspect of using ICTs to enhance learning.

An activity's design should depend on its goals. Gregorius suggests that goals can determine when to apply behavioristic, cognitivistic, and social constructed or situated learning perspectives. If an animation was designed to promote learning in nomenclature and balancing equations, then digital games and drills that enhance rapid response skills in a behaviorist fashion would be appropriate. If the goal shifts from rapid response to the method by which an answer is obtained, then the design needs to be interactive and based on cognitivist research. What the learner brings to the lesson guides situated learning activities, which should be tunable to the learner's "zone of proximal development". The activity should be at the fringe of what the learner can do without guidance. Gregorius also presents design parameters for developing multimedia; these are based on Mayer's work on cognitive load and dual-coding theory. Finally he introduces the Inductive Concept Construction (IC2) Learning System, an eBook that utilizes these concepts.

It is clear that no matter what methods or tools are used for instruction, a major challenge is to identify a student's zone of proximal development and then provide lessons tuned to it. By mating digital technologies with knowledge space theory, it is possible to create a knowledge map and identify an individual's knowledge state within a knowledge domain. This effectively identifies the zone of proximal development and allows lessons to be generated on a student's knowledge fringe.

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In their chapter, "Reaction Explorer: Towards a Knowledge Map of Organic Chemistry To Support Dynamic Assessment and Personalized Instruction", Chen et. al. describe development of *"Reaction Explorer: Organic Chemistry Tutorials"* (*23*), which is now distributed commercially via WileyPLUS. This rules-based program uses 1,500 reaction rules as knowledge items from which a knowledge map is created in the domain of organic synthesis and mechanisms. The authors then describe how they create a knowledge state model by assessing a student's success/failure rate solving problems. The model is based on knowledge items associated with a problem, and on associations and dependencies of those items. It allows them to predict the probability that a student can solve a new problem. A directed problem selector can then generate problems on a student's knowledge fringe, which is effectively the zone of proximal development.

What are the challenges and rewards of offering a course online? How does one go about designing such a course? Can an online course be successful? Tomasik and Moore answer these and other questions in "Site Under Construction: Designing a Successful Online Course". As part of the education/outreach program for the NSF-sponsored Nanoscale Science and Engineering Center (NSEC) at the University of Wisconsin−Madison, the authors designed and offered an online course, Nanoscience for Teachers. The purpose of the course, which was initiated in 2006 and continues to be offered, was to provide high school teachers with appropriate background in nanoscience and nanotechnology and to encourage them to include nanoscience topics in their courses. In both of these regards the course has been successful: teachers have created units on nanoscience, used them with students, and shared them with other teachers.

One challenge faced by those offering online courses is that unless the course is well designed the student dropout rate may be greater than in a similar face-to-face course. This depends in part on the course content, how the content is presented online, the means of communication among participants and with the teacher, and the degree of interactivity the course structure affords. During early offerings of the online nanoscience course, these aspects were explored through formative assessments and the course design was changed accordingly. Steps were taken to assure high quality interactivity of participants with the course content, with the instructor, and with peer students. Interactivity included: weekly chat sessions with practicing nanoscientists; online forums for discussion among students, teachers, and experts in nanoscience and peer review by course participants of the lessons being developed by other course participants.

Another challenge is obtaining content that can be used without violating copyright. The authors emphasize that course designers must consider copyright with respect to all content and work with librarians and others knowledgeable in this area. Fair use is not a simple subject and different universities and school systems may have different interpretations of what is and is not appropriate. In the case of Nanoscience for Teachers, it was often possible to use materials that were copyrighted but that had been licensed for use by all students by the university offering the course. This license extended to students whether or not they were physically on campus because access to the course was restricted by the course management system (Moodle) within which the course was developed.

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Finally it is crucial that an online course undergo continual formative evaluation. Both the tools available to course designers and the expectations of student participants are continually changing. So are the copyright permissions for content and fair use. What works one year may not work the next. The equivalent of dog-eared lecture notes is not an option—which may be another advantage of an online course!

This section deals with a general view of the options available to those designing online course materials and how learning theory and chemical education research can be applied to an online course and its components. We hope it provides insights that will improve online courses and that it encourages readers to develop their own online courses or course components.

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Part IV: Digital Libraries: Creating, Refining, Storing, and Disseminating Online Resources

What is a digital library? Why should I use a digital library? The name "digital library" connotes similarity to a traditional library: That is true in the sense that a digital library is a collection of online items that can be used for research and to support learning, but digital libraries have many more dimensions. For example, when NSF's National STEM Digital Library (NSDL) project (http://nsdl.org/) was initiated in 2000, it began by collecting and cataloging online content for both education and research. So that each item could be retrieved easily NSDL assigned metadata keywords and operated a search engine that located resources by keyword. During its decade of existence, however, the NSDL has continually expanded its scope and facilities and identified new directions in which it needed to move to serve its constituencies.

The NSDL's collections in chemistry, held by the Chemical Education Digital Library (ChemEd DL, http://www.chemeddl.org/), are typical. They include a broad range of content: many hours of streaming digital video showing chemical reactions, apparatus, and laboratory techniques; quiz and examination questions including multimedia that can be delivered via Web-based course management systems; and Jmol molecular and crystal structures that can be manipulated with a mouse and that can display molecular orbitals, vibrations, symmetry, and other properties. The NSDL and its constituent groups such as ChemEd DL also serve as curators of the collections, keeping the content current. This involves dealing with issues such as URL rot, updating video and other content to meet new standards, and modifying content for dissemination via new modalities such as smartphones or iPads.

NSDL's creation in 2004 of Pathways projects—a means of tailoring the NSDL to serve the needs of a specific discipline or some other well defined audience—is an example of its continual evolution. In 2010, ChemEd DL is one among nearly 20 NSDL Pathways. The Pathways represent most scientific disciplines, groups such as public broadcasting and science museums, and audiences at specific educational levels, such as middle school or two-year and community colleges. A new Pathways project was initiated in 2010 that will concentrate on aiding teachers and school districts to incorporate NSDL resources into courses and curricula. Through its many specialized Pathways, NSDL serves as a focus for communities that are creating and using online teaching and learning materials, as an aggregator of individual learning objects into larger modules that can be used by teachers and students to teach sizable portions of content, and as a national group that can work with state education agencies and individual school systems as well as teachers to bring highly effective online resources to students from K-16 and beyond. This broader scope has resulted in a change of name (but not abbreviation) to National STEM Distributed Learning.

The importance of digital libraries in furthering educational goals is nicely exemplified by several chapters in this book. “Instruction Online: Core Components for Re-Use” by Yaron et al. describes the ChemCollective digital library and illustrates how online instructional materials from this project have been created and continually improved by a community that involves programmers, instructional specialists, content experts, and users (teachers and students). The authors contend that digital libraries can contribute to fundamental changes from existing instructional techniques, resulting in significant improvements in learning. They can do this by building and encouraging communities to develop and try new approaches, and by providing the means online by which members of such communities can evaluate and incrementally improve the new approaches. This requires use of technologies that enable relatively quick and easy modification of instructional materials by people who are not expert in information technology.

Some examples of materials in the ChemCollective digital library are the Virtual Laboratory collection, a stoichiometry course, an equilibrium course, and Core Ideas in Molecular Science (CIMS). The Virtual Laboratory provides a means for students to do simulated laboratory work online much faster than it could be accomplished in a wet laboratory. In addition, the entire community of users can modify and improve experiments through the digital library interface. The online stoichiometry course provides a means by which students anywhere in the world can review what is perhaps the most important fundamental chemistry skill—one that many other disciplines count on general chemistry courses to teach well. The ChemCollective equilibrium course illustrates a different approach to teaching this important topic—an approach that has more than doubled student performance. CIMS is a collection of interdisciplinary instructional modules that have been tailored to specific disciplines as a means of encouraging teachers in each discipline to use them. One module, for example, uses molecular-scale animations to teach the ideas of energy, entropy, and Gibbs energy as applied to chemical equilibrium. All of the items in the ChemCollective have benefitted from honing by users and by those from other disciplines in different NSDL Pathways.

“Developing ChemPRIME: Transforming the Didactics and Pedagogy of the General Chemistry Course with a Wiki Text” by Ed Vitz is another illustration of the usefulness of digital libraries. ChemPRIME (Chemical PRinciples through Integrated Multiple Exemplars) combines an idea that is more than a decade old (but nearly impossible to achieve at the time it was conceived) with the power of a wiki on a server operated by the ChemEd DL. The idea is that many students would be attracted to chemistry if they could see more clearly how chemistry is

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applied in the fields of their primary interest, but that it is also beneficial to retain a logical structure for chemistry as a discipline so that students can appreciate the relationships among chemical facts and theories. A wiki is ideally suited to storing and serving alternative approaches that illustrate applications of chemistry topics in a variety of fields; a wiki also enables a broad range of teachers (and even students) to contribute such alternative approaches. ChemPRIME applies this approach to the general chemistry course.

Many academic degree programs, such as engineering, biology, pre-medicine, computer science, physics, or geology, require general chemistry—and for good reasons. However, it is not clear to students that the considerable time and effort they spend on studying general chemistry reflects the actual benefit they will gain. Benefits would be more obvious if each discipline had its own chemistry course that was fine tuned to the needs of that discipline. This would allow students to learn via exemplars from the discipline of their choice and within the context of their interests. Realistically, however, even a large school cannot afford to offer the number of general chemistry courses that would be required to accommodate all student interests. Typically general chemistry instructors use a textbook for chemistry majors, which cannot promote students' sense of the importance of chemistry to their disciplines nearly as well as a textbook fine-tuned to their major.

ChemPRIME has scanned, digitized, and converted to wiki format a typical general chemistry textbook, "Chemistry" by Moore, Davies, and Collins. This wiki textbook provides a complete treatment of the content usually encountered in a general chemistry course; in the wiki this is called "CoreChem". Ten "tracks" are being created parallel with the CoreChem, representing interests ranging from chemistry in everyday life to chemistry in physics and astronomy. Each track consists of many exemplars; when complete, the wiki will contain one or more exemplars in each track for each CoreChem topic. The wiki enables a variety of authors to enter exemplars into each track. Usually they begin with the CoreChem topic and then apply the concept to the track's subject area, fine-tuning the presentation and examples to the other discipline. Thus each of the ten tracks teaches the same concepts as CoreChem, but each embeds the concept in the context of another discipline or area of student interest. Consequently students in environmental science, geology, or biology would all learn about heat capacity, and all would learn through exemplars that were relevant to their interests. A wiki allows this to be done in a dynamic way by having participants in the general chemistry community contribute exemplars in their areas of interest. Contributors to the wiki become members of a general-chemistry community in the digital library.

The wiki format of ChemPRIME affords a teacher great latitude in specifying which topics should be studied in what order. Students also have great latitude in deciding which tracks or exemplars to study. But the wiki is not ideally suited to presenting an online textbook in the most approachable format. A wiki is dynamic—changing whenever someone edits an entry—and navigation in a wiki is limited. "The ChemPaths Student Portal: Making an Online Textbook More than a Book Online" by Shorb and Moore describes a digital-library service of the ChemEd DL that addresses the problems of wiki-based content. ChemPaths enables a teacher to specify a path through the wiki content and restrict the content

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to a snapshot of the wiki taken at a particular time. Thus the order of presentation of the content can be structured as a teacher desires (for example, atoms first or chemical reactions first), and the content remains unchanged during a course. ChemPaths can be likened to a path of stepping stones with other shorter paths off to the side. It enables a student to follow the order of topics in CoreChem, for example, but to deviate to exemplars in one or more other tracks and then easily return to the main CoreChem path. Or a path could be specified that involves a track as the main focus, and a student could explore CoreChem as one possible side-trail.

ChemPaths enables a variety of pedagogical approaches that are not available in a printed textbook. Thus teachers need not all adopt the same approach to designing what students will see when studying a given topic. The interface design of ChemPaths was based on research in hypertext learning and visual learning. It combines interactive molecule viewers (Jmol), embedded videos, and animations with explanatory text, affording students multiple representations of the same concept. Students can obtain definitions of terms by mousing over words, and links are provided to topics closely related to the one being studied. A periodic table, data tables, and the table of contents of CoreChem are always a mouse-click away. Online quizzes provide feedback including links to the relevant sections of the online textbook. This chapter describes the theories from which the design was derived and how an integrated learning system was developed for online delivery.

This learning system has been tested in courses enrolling hundreds of students. Student feedback was obtained both during a course and at the end, and such feedback has led to changes in the delivery system as well as how students are introduced to it. Questions that had to be addressed include: accessibility for students with disabilities; means by which students can annotate, highlight, and bookmark text; organization and presentation of content and navigation; and students' skills in using online materials compared to printed materials. The authors found that it is useful at the beginning of a course to introduce students to techniques for using an online textbook and even to provide a quiz or tutorial that prompts students to explore and use various features of the online medium. It is apparently a fallacy that all students are familiar with and comfortable with an online delivery system. There is almost certainly a lot more for us to learn by observing real students in a real course as they interact with this new learning aid.

In "Building an Online Teaching Community", Reisner et al. describe another aspect of digital libraries: building a community and providing for communication among its members using Web 2.0 tools. They describe the growth of the Interactive Online Network of Inorganic Chemists (IONiC), a community of practice, and IONiC's development of a Web interface and online repository, VIPEr (Virtual Inorganic Pedagogical Electronic Resource). The authors, who are mostly from primarily undergraduate institutions, state at the beginning, "We never set out to build an online community." But they did set out to communicate, spurred by the fact that in the smaller colleges where most of them teach there is usually only a single inorganic chemist—who yearns for professional discourse with others who have similar interests. The formation of IONiC came at a fortuitous time, because Web 2.0 technology was becoming available that

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enabled much richer communication: videoconferencing, cloud-based workflows, long-range collaborations, and close personal relationships.

One aspect of VIPEr that perhaps runs against the grain for many who are used to the traditional submit, review, evaluate, publish or decline process of peer-reviewed journals is the relative ease of posting materials. A post must be approved by a member of the leadership group, but then it is released to the public and the review process occurs post publication. Often a review consists of comments from users of the material and is based on actual classroom use. This is a sensible way to get thorough evaluations but does not carry the cachet of a peer-reviewed journal. This is an aspect of publication that is worthy of considerable thought and debate. Is prior peer review necessary and desirable in a world where it is easy and convenient for any user to post a review after publication? Will enough users of materials be willing to take the time to contribute reviews and comments, no matter how easy it is? Will tenure committees accept and approve of a process of publication followed by review?

Building the IONiC/VIPEr community benefitted from several factors: an enthusiastic, actively communicating leadership; a latent need for communication; demonstrable benefits that maintained momentum; occasional face-to-face meetings; a medium for sharing information that is easy to use; commonality of interests combined with breadth of membership; a community that is big enough, but not too big; and a collective sense of humor, a mascot, and lots of fun. The online community that IONiC has created exemplifies all of these characteristics. This chapter is a must-read for anyone who aims to create a community of any kind, because it contains a great deal of wise counsel. More important, it is just fun to read!

Like the Web itself, the digital library is a constantly evolving work in progress. Like all digital libraries, the NSDL, the ChemCollective, IONiC/VIPEr, and the ChemEd DL have evolved significantly since their inception. They will evolve even further in the future, as new tools become available to facilitate storage, retrieval, and use of high quality online instructional materials, to enhance communication and community building, and to provide new means by which student learning can be encouraged and expanded. Stick around. The fun has just begun!

Part V: Looking Ahead

Despite the wide variety of the techniques discussed in this book, the editors clearly understand that not every important development in instructional technology has been covered. This is not due to any lack of ability or foresight on the part of our contributors, but rather due to the massive and rapid nature of the changes that are currently happening. The educational process is being reshaped not just by the developments reviewed in this book, but also by new software and new devices. There are several such topics which we hope to cover in future ACS symposia, online conferences such as ConfChem (*24*), and subsequent volumes of this series.

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Pioneering work in several areas is ongoing. Cloud computing, where software does not reside on the local computer but is accessed through the World Wide Web, promises new opportunities for collaboration and organization (*25*). A few audacious teachers have demonstrated that virtual worlds, like Second Life, can be an effective venue for chemical education (*26*). The social networking applications that have grown so rapidly over the past decade can also have real value for learning. eTextbooks will probably become increasingly important in the future, but there is also a strong possibility that content will become disaggregated and learning modules may become a supplement or replacement for textbooks (*27*). Online learning seems to be generally accepted by educators, and there is increasing interest in hybrid approaches that combine online activities with the traditional classroom. Distributed and transmedia narratives are creating new types of literacies that our students need to understand.

Digital electronic devices are proliferating faster than a book can keep up. They continue to become faster, smaller, and cheaper, creating a succession of new educational capabilities. An obvious example is the ubiquitous cell phone, which has become a powerful handheld computer with Web connectivity. Many people take these devices with them everywhere, creating a 24/7, always-on world of virtual information accessibility. It remains to be seen how these might best be used for education. These "smartphones" are combining with augmented reality to create a whole new range of applications for the chemistry classroom (*28*). The popularity of the Apple i-Pad is already inspiring a plethora of clones, which may well make gesture-controlled navigation the standard computer interface of the future. The Microsoft Kinect is designed to be a game system, but developers are already creating scientific applications (*29*). If the Kinect redefines the way humans interact with computers, there is little doubt that it will also have a significant effect on education (*30*).

Some suggest that the rapid rate of change argues for teachers to wait until stability is reestablished before investing their effort on new technologies. This is not a viable strategy. The pace of change is accelerating, and there is a real need for broad-based experimentation to explore the pedagogies that must be developed to make full use of the new educational environment. Although it is impossible for a single individual to try all of the technologies, it is hoped that the chapters in this book will encourage many teachers to try individual techniques that appear most useful to their needs. Now is the time to explore new ways to support and foster student learning.

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Chapter 2

ChemSpider: Integrating Structure-Based Resources Distributed across the Internet

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Accessing information about chemicals distributed across the Internet is, in many ways, too easy. Chemists simply type in the name of a chemical of interest into a search engine and then wade through the results hoping to find a result matching their query. Such approaches are limited to the whims of text-based matching and it can be very time-consuming to wade through pages of results attempting to segregate the various types of information retrieved. ChemSpider is a free online structure database developed with the intention of aggregating and linking chemical structure based information and data across the Internet. Containing almost 25 million unique chemical entities and linked out to over 300 data sources ChemSpider offers the ability to perform *both* text and structure-based searches to resource information such as chemical vendors, properties, analytical data, patents, publications and a myriad of other information. While enabling this broad form of searching for chemical data across the Internet ChemSpider has also assumed a key role in allowing the community to expand and improve the online data by providing a platform for community deposition, annotation and curation. As a result the ChemSpider Web site has become a crowdsourcing environment for chemists to expose their own activities to the community and participate in creating the richest single resource for chemistry related information available online and, in keeping with the nature of the Web, for free.

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
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Introduction

The Internet has forever changed the way that we will search and access information. The departure from software resident on a local computer to Web-based interfaces and computation and storage in the cloud is quickly blurring the lines between software we own and functionality and systems we access. This is even more prevalent in the domain of access to data where online resources and search capabilities have become the dominant manner by which we resource information. Google has become a *verb* rather than just a search engine. Wikipedia has become *the* encyclopedia of the modern age. For chemists there are an abundance of resources available online served up by chemical vendors, publishers, government databases, grant-funded academic databases, commercial systems and many other forms of data. Using these resources, and powered primarily by the *de facto* search engines of Google, Yahoo and now Bing, chemists can research information about their specific area of chemistry and generally can find information of relevance to their search. It is a new world of data access. It is also a new world of contribution where chemists can contribute directly to the data and information available online.

Web-based technologies coupled with a drive for improved communication between scientists has resulted in the proliferation of scientific opinion, data and knowledge at an ever-increasing rate. The availability of tools to host wikis and blogs has provided the necessary building blocks for scientists with only a rudimentary understanding of computer software science to communicate to the masses. This newfound freedom has the ability to speed up research and sharing of results, develop extensive collaborations, conduct science in public, and in near-real time. Communication in chemistry is witnessing a new revolution.

In recent years a number of efforts have been made to deliver so-called "public compound databases" to the community containing anywhere from a few hundred to many millions of chemical structures with associated information. These can vary from databases with a specific focus, for example metabolites or pesticides, or can simply be information aggregators or repositories where data are aggregated *en masse*. Databases built with a specific focus in mind are generally quite small, a few hundred to thousands of compounds only, highly curated, painstakingly assembled and developed with a particular class of chemists in mind. Data aggregators and repositories are commonly much larger, tens of thousands to millions of compounds, and are holders of data which are contaminated with numerous errors and, while easy to search, can commonly deliver misleading results. The Internet therefore hosts information that is hard to filter, difficult to segregate and, at best, challenging to interpret in terms of quality. At a time when some students function with the mindset that if it is not on Google it does not exist, and where Wikipedia is fast becoming the primary reference work for much of their online searching, there is a need for a sincere effort to improve and distinguish the quality of online information for chemists. This article will focus on our efforts to build the *de facto* online resource of chemical compounds, syntheses and related data linked out across the myriad of Internet resources, both open and commercial. We will examine how such resources can offer benefits to students and educators to delve into Cheminformatics, online searching and data validation and how access to such a system can speed and support research.

Cheminformatics in Education

Ask a chemist how often they use the Internet to search for data and information online and nowadays one would expect the answer to be “many times a day”. The Web is now the primary portal to query for general information and data. Bioinformatics led the charge to provide online access to data with open-access databases such as GenBank (*1*) and the Protein Data Bank (*2*). Biologists have been using these resources to translate gene and protein sequences into biological relevance for well over two decades. In recent years chemists have pursued their own activities to provide free and open access to chemistry-related information. The progress in the availability of freely-accessible information is highly enabling and advantageous for the advancement of science. Pharmaceutical companies in particular welcome improved access to chemistry-related information as their business dominance is endangered by drugs coming off patent when no replacement blockbuster drugs are in the pipeline.

Just a few years ago the majority of students completed their education with the intention of entering a career in chemistry were likely ill-equipped to take advantage of the cheminformatics tools, databases and tools that they would need to understand when they entered an organization. The reasons were primarily those of cost and availability. Most cheminformatics tools were expensive and unavailable to students while searching was limited to library review of paper-bound journals and abstracts and consultation with librarians to perform their searches. Today students have access to a multitude of open source or free chemistry software packages, free access online chemistry databases, simple online interfaces for searching articles and, Internet search engines that can search for literally anything of interest to them. Commercial vendors of software tools and systems commonly offer price points to the educational institutions to make their software affordable and accessible and students will generally leave their training institution with a reasonable appreciation of what is available and expected of them when they are gainfully employed. Nevertheless, there are very few institutions with training courses dedicated to Cheminformatics per se despite the fact that a grounding in chemical structure handling, online and database searching and the application of software tools for molecular modeling or property generation would likely be of benefit to their graduates in their careers. It is this author’s belief that the Internet can now deliver access to the majority of tools that could form a foundation of technologies that students need to understand.

Learning to use chemical structure drawing software is an essential skill for all chemists during their education as it is the basis of input to chemistry search systems to retrieve publications, patents and data. An ability to sketch a chemical structure or define a substructure to perform a substructure search is not difficult to develop and any student can download, free of charge, a number of structure drawing packages. These packages generally include 3-D structure optimization routines, rudimentary or advanced nomenclature generation and

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property generation routines. They include algorithms for the generation of other structure representations other than those of aesthetically pleasing visual depictions of molecules—these are, for example, SMILES strings (*3*) and InChIStrings or InChIKeys (*4*) that are commonly used for searching databases, linking resources and enabling Internet chemistry. All students should have an exposure and grounding in these basic tools and terminologies.

A students' familiarity with computer-based data processing should have been developed via the application of statistical analysis of data, utilizing data systems for the acquisition and manipulation of, for example, chromatographic or spectroscopic data, and using desktop tools such as Excel or other spreadsheet packages. Experience in these areas is expected now by all employers.

A student will hopefully have access to one or more of the chemistry database systems including systems such as CAS Scifinder (*5*) or Elsevier's Reaxys (*6*) system. These resources enable a user to perform both text and structure/substructure based searching of millions of articles, patents and reactions using quite standard querying approaches and the development of skills in this area will be of very high value for their future careers. Unfortunately, access to such tools may be limited to library-only based access, some of these resources are expensive, and the license concurrency limits usage and availability. To complement these commercial programs, students should be aware of the many resources available online. This will be the focus of the next section in this chapter.

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Resourcing Chemical Data Online

The success of Internet search engines is driven primarily by the willingness of all participants and contributors to the Internet community to allow their sites to be indexed in order to become more discoverable. Any individual or organization posting data (photos, music, spectra, text, publications, etc) to the Web is likely doing so with the intention that it will be indexed and discovered. The majority of companies expect to trigger a transaction as an outcome which can be revenue or reputation generating. For chemistry this may be the sale of a chemical or piece of apparatus, the purchase of access rights to the PDF or Web-based form of an article, access to data within a database and so on. While some of the resources online are able to commercially capitalize on the transaction resulting from a search, the majority of data now available online is free to access. Enormous investments have been made by funding bodies to provide infrastructure, make data freely available and enable research. Open Access, free access and author pay models for publishing has resulted in unprecedented access to the scientific literature. Learning to locate, search and navigate the Internet to investigate these resources is a valuable skill for any scientist.

There are literally hundreds of online chemistry databases containing chemical compounds, reaction syntheses, property data, spectral data, genomics data, protein structures, metabolism maps, chemical vendor collections and so on. An effort to list all such available databases would be incomplete and out of date by the time this article was published.

A number of specific databases will be briefly mentioned but the reader is referred to an article by this author regarding Public Compound Databases that offers a more detailed examination of this domain (*7*). The short selection demonstrates that online compound databases can allow searching of chemicals, biological assay data, links between chemical and biological data including genes and proteins, links into both publications and patents as well as into the opinions and activities of individual scientists via their Weblogs.

The PubChem database (*8*) was launched by the National Institutes of Health in 2004 as part of a suite of databases to support their roadmap initiative (*9*). PubChem archives and organizes information about the biological activities of chemical compounds and is intended to empower the scientific community to use low molecular weight chemical compounds in their research. PubChem consists of three databases (PubChem Compound, PubChem Substance, and PubChem Bio-Assay). As of May 2010 its content is approaching 68 million substances and 27 million unique structures but provides biological property information for a fraction of these compounds. PubChem can be searched by alphanumeric text such as chemical names, property ranges or by structure, substructure or structural similarity. The system has an important role as a central repository for chemical vendors and content providers enabling evaluation of commercial compound libraries. The system provides descriptions of chemicals and links to PubMed (*10*), over 19 million citations from MEDLINE and other life science journals for biomedical articles back to the 1950s. Zhou *et al.* (*11*) examined the intimate relationship between PubChem and PubMed and at the time of their study showed that there were over 82,000 PubMed papers and 1.6 million PubMed Central papers linked to PubChem. Numerous scientists have commented regarding the quality of the data content within PubChem. Screening data are less rigorous than those in peer-reviewed articles and contain many false positives (*12*). Deposited data are not curated, and so mistakes in structures, identifiers units and other characteristics can, and do, occur. The author of this article has pointed to the accuracy of some of the identifiers associated with the PubChem compounds (*13*, *14*). The problems arise from the quality of submissions from the various data sources. There are thousands of errors in the structure-identifier associations due to this contamination which can lead to the retrieval of incorrect chemical structures. It is also common to have multiple representations of a single structure, due to incomplete or total lack of stereochemistry for a molecule.

DrugBank (*15*) blends both bioinformatics and cheminformatics data and combines detailed drug (*i.e.* chemical) data with comprehensive drug target (*i.e.* protein) information. The database contains >4800 drug entries and >2500 protein or drug target sequences are linked to these drug entries. Each DrugCard entry contains almost 100 data fields, with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data.

The group hosting DrugBank also provide access to a series of other curated databases: the Human Metabolome Database (*16*) contains detailed information about small molecule metabolites found in the human body and is used by scientists working in the areas of metabolomics, clinical chemistry and biomarker discovery. They also host the FoodDB (*17*), a comprehensive database providing information

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on over 1900 food components, based on the FDA list of everything added to food in the United States.

SureChem (*18*) provides chemically-intelligent searching of a patent database containing millions of US, European and World Patents. Using extraction heuristics to identify chemical and trade names and conversion of the extracted entities to chemical structures using a series of name to structure conversion tools, SureChem has delivered a database integrated to nearly 10 million individual chemical structures. The free access online portal allows scientists to search the system based on structure, substructure or similarity of structure, as well as the text-based searching expected for patent inquiries.

Wikipedia (*19*) is an unprecedented success story in the domain of community intellectual contribution and crowdsourcing. For chemistry it represents an important shift in terms of the future access of information associated with small molecules. A wiki is a type of computer software allowing users to easily create, edit and link Web pages. For small molecules on Wikipedia each one generally has a Drug Box or a Chemical infobox. The drug box shows a chemical identifier, one or more chemical names or identifiers, links out to related resources, chemical and pharmacokinetic data and therapeutic considerations. At present there are approximately 10,000 articles with a chembox or drugbox. The detailed information offered on Wikipedia regarding a particular chemical or drug can be excellent or weak in the case of stub articles (a stub article is an article that has been started and is awaiting expansion). There are many dedicated supporters and contributors to the quality of the online resource. This community curation process makes Wikipedia a very important online chemistry resource, whose impact will only expand with time. The author of this article is part of a dedicated team who have worked on validating and curating Wikipedia chemical compound pages for over two years (*20*).

An increasing number of scientists have an urge to publically communicate about either their own science or science in general, commonly with the intention of educating others, proliferating data or opinions, or connecting with others for the purpose of collaboration or advice and both wikis and blogs are fast becoming chosen platforms for the exchange of information between many scientists (*21*). There are blogs from members of the pharmaceutical industry, from the cheminformatics world, from the open source chemistry software world and other willing participants in the "blogosphere", specifically students.

The short list discussed above is meant to be representative of the types of resources that are becoming increasingly available online as individuals, researchers and organizations contribute to the data available via the Internet. In order to provide a unified approach to searching across these multiple diverse resources via a single search engine ChemSpider was developed.

ChemSpider: A Structure Centric Hub for the Internet

ChemSpider (*22*) was initially developed as a hobby project by this author and a small team of voluntary programmers as a free offering to the chemistry community. ChemSpider is built primarily on commercial software using a

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Microsoft technology platform of asp.NET and SQL Server as this allowed ease of implementation, projected longevity and made best use of available skill sets. Following a short development cycle of just a few months ChemSpider was released to the public in March 2007 with the lofty goal of "building a structure centric community for chemists".

ChemSpider has since grown into a resource containing almost 25 million unique chemical structures linked to over 400 original data sources. Data have been aggregated as a result of contributions and depositions from chemical vendors, commercial database vendors, government databases, publishers, members of the Open Notebook Science community (*23*) and individual scientists (*24*). The database can be queried using structure/substructure searching and alphanumeric text searching of both intrinsic, as well as predicted, molecular properties. Various searches have been added to the system to cater to various user personae including mass spectrometrists and medicinal chemists. At this time the search system is both flexible and fast. A screenshot of the interface is shown in Figure 1.

Following the deposition and aggregation of the data from a multitude of data sources it became obvious that one of the side effects of such an activity was that data of various levels of quality were being merged. In order to provide a trusted resource there was a clear and obvious need for data curation and validation. Since the ChemSpider team was both small and voluntary there was no easy manner by which to perform data validation without engaging the community directly with a request to provide crowdsourced support of the project. A project was therefore undertaken to enable real time curation of the data. The social community aspects of the system demonstrate the potential of such an approach. Real-time and rules-based curation of the data has resulted in the removal of hundreds of thousands of incorrect identifiers and the creation of a large validated name-structure dictionary containing well over a million identifiers. Such a validated dictionary can be important to providing high precision for chemical name entity extraction as reported by Hettne *et al* (*25*).

Following the addition of community-based curation, facilities were added to enable further annotation and expansion of the data. Features were added to allow the association of analytical data with chemical structures, real-time deposition of single or batches of chemical structures and transaction-based predictions of physicochemical data. As a result of contributions from scientists supporting the vision of ChemSpider as a valuable centralizing community-based resource for chemical data for chemists, almost 3000 spectra have been added to ChemSpider in the past 2 years with additional data being added almost daily. These data include infrared, Raman, mass spectrometric and NMR spectra with the majority being 1H and 13C spectra. These spectra are the foundation data for the development of a spectral game to assist in the teaching of NMR spectral interpretation (*vide infra*).

The motivation behind the ChemSpider platform was one of providing an environment for collaboration and ongoing community contribution for the expansion of the data and knowledge supported by the database. While Wikipedia is likely one of the standards in terms of community participation for curation and authorship the platform is not chemically aware in an informatics sense with the absence of quite basic capabilities such as structure and substructure searching. At the other extreme PubChem is advanced in an informatics sense but is non-curated and offers little opportunity for a chemist to do more than use the system. ChemSpider was always intended to be a gathering place for chemists to utilize an advanced cheminformatics platform for adding, curating and enhancing structure-based information. As a result of its successful immersion into the chemistry community, and an aligned common vision of supporting chemists in their research, the Royal Society of Chemistry (RSC) acquired ChemSpider in April 2009 (*26*). The vision of developing a community portal for chemists to source data and information has remained and in June 2010 ChemSpider was awarded a Best Practices Award by Bio-IT for its community service (*27*).

Since joining RSC ChemSpider has initiated a path to integrate RSC content into the database. RSC developed an award-winning semantic markup project known as Project Prospect (*28*). “Prospected” articles incorporate standard metadata within the full text of their articles and combine this with an intuitive on screen manifestation of the advantages of including this metadata. For chemists this translates to a number of features including the display of compound pages showing the chemical structure, various identifiers and links to other online resources when hovering over a chemical name with the mouse cursor. Chemical structures which are prospected in the articles are now deposited directly into ChemSpider on an ongoing basis together with a direct link back to the associated article. This makes RSC articles more discoverable and provides direct benefits to the reader of the article as the compounds are linked into the ChemSpider database thereby opening up access to an expansive set of data and links across the Internet.

To date ChemSpider has provided integrations to structure linking from the ChemSpider database into the RSC Publishing archive of over half a million articles as well as links into RSC Books and RSC Databases (*29*). The manner by which this integration has been performed is to use an application programming interface on the RSC Web site to search *validated* chemical identifiers (systematic names, trivial names, registry numbers etc) using a text query. The result is a fast and efficient search providing direct links to the relevant data contained in the RSC Publishing database. A similar approach has been taken to integrate to Pubmed, Microsoft Academic Search, Google Books, Google Scholar and Google Patents. Such an approach has literally made the entire Google content structure searchable via ChemSpider (see Figure 2 for an example). A chemist can now draw a structure on ChemSpider and retrieve books, articles and patents served up by the world’s most well know search engine in just a couple of seconds. Most importantly the access to all of this data is free.

What ChemSpider is to the delivery of information and data for chemical compounds ChemSpider Synthetic Pages (CS|SP) (*30*) intends to provide to chemists in regards to reaction syntheses. There is one caveat however—the community is fully responsible for populating each record in the database, as CS|SP is primarily a publishing platform for chemists. While there are many commercial reaction databases, there is no free database of synthetic routes that the community can comment on, populate and expand. CS|SP is a derivative work of the original SyntheticPages project. In a joint collaboration RSC-ChemSpider and the SyntheticPages team have delivered a new architecture for the hosting of

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synthesis procedures and enhanced the original data model such that the platform can now host multimedia content, spectral data, allow semantic markup and linking to the ChemSpider database and most importantly, enhanced capabilities for the deposition of synthesis procedures and data by members of the community. A screenshot of the CS|SP home page is shown in Figure 3.

CS|SP is envisaged to be a manner by which chemists, and students specifically, can grow a professional online reputation for themselves as synthetic chemists. Each SyntheticPage has a single author, the chemist who performed the synthesis. The lab head or supervisor is credited via the association of the synthesis with a particular research group. Following submission a SyntheticPage proceeds through a review process by one or more members of the editorial board made up of five academic synthetic chemists (*31*). Feedback is provided to the author if necessary and edits can be made online. When the SyntheticPage is published then the community can then provide direct feedback in terms of additional questions, comments regarding their own experiences of repeating the synthesis, alternatives to the reported synthesis and so on. In this way this community research becomes an engaging dialog between synthetic chemists as well as representative of their skills and activities. Each SyntheticPage will receive a digital object identifier (DOI) (*32*) and will make a valuable addition to a resume. As of July 2010 the database hosts almost 400 synthetic procedures with new submissions being made on a regular basis. The intention is to engage the community to participate in the further development of this rich resource for chemistry. It is intended that the RSC archive will also be tapped for previously reported syntheses which could be added to the database.

ChemSpider SyntheticPages offers an interesting opportunity for students and learning. Authoring a publication and passing through the peer review process can be an overwhelming task for a student. For the normal publication process through a classical scientific journal there is certainly no guarantee of success, a publication can be an enormous undertaking and peer review is anonymous and slow. Learning to report scientific data and process in sufficient detail to garner the approval of peer reviewers, and then publishing this information to the public domain to gather input from online readers provides the student contributor to CS|SP a reduced yet valuable experience in the preparation of scientific documentation for peer review.

Using the content on ChemSpider as a foundation Bradley *et al.* have set up an online game to learn how to interpret NMR spectra. The Spectral Game (*33*, *34*) has already been played by thousands of students around the world. The game uses a Web service supplied by the ChemSpider database to serve up spectral data and associated chemical structures. Users log in to the game to keep track of their scores. At the beginning of the game two structures, one correct and one incorrect are shown below the spectrum, see Figure 4, and the user is asked to click on that structure that is the best match for the spectrum displayed.

The player needs to examine the spectrum to compare various features to confirm or reject each of the structures. These include shifts, multiplicities, peak intensities, functional groups and so on. In NMR users should be able to quickly distinguish aromatic protons from alkyl protons, aldehydic resonances from exchangeable carboxylic acid protons and methoxy singlets from methylene groups within a chain. The game becomes increasingly difficult with the number

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of associated structures increasing, to a maximum of five per spectrum. As the number of structures increase they also become more structurally similar. When a player reaches a score of forty, rounds also become timed, and the player must select an answer before the countdown expires. The amount of time a player gets decreases as rounds progress to a minimum of ten seconds.

Playing the spectral game immerses students in the process of spectral validation rather than structure elucidation and spectral assignment. Players are engaged in the common process of checking for consistency between the spectral data and structures, using the phenomenon of chemical shift, couplings and basic integrals to determine the appropriate relationship between the structures and the spectrum. Spectral assignment is a deeper process requiring establishing the absolute relationships between the various spectral features and the magnetically active nuclei in the molecule of interest. Structure elucidation is a different process again requiring the elucidation of a total unknown from the displayed spectral features.

One of the side benefits of the Spectral Game is the examination of the data and reporting of potential issues to the hosts of the game. As players progress through the game they can flag spectra initially displayed in reverse and leave comments associated with each of the spectra. Then, curators on ChemSpider can review the data and take the appropriate actions. The percentage of time that a spectrum is matched correctly is also recorded giving a measure of how "difficult" the spectrum is to interpret. In the year since it has been online the game has had >8000 unique visitors from >80 countries and over there have been well over 100,000 spectral views during that time.

The NMR data within the game have been harvested from various Web sites and deposited by users of ChemSpider. In order to deposit a spectrum a user simply searches ChemSpider for the associated structure, uploads the JCAMP-DX spectrum and it is available to the community immediately. The data base grows only as a result of participation by the community. A 2-D NMR Spectral Game is available as a proof of concept (*35*). 2-D NMR, while generally used less in education than the standard 1D spectroscopic methods is a necessary skill set to develop for a synthetic organic chemist.

There are more complete educational tools available online for students to access to learn more about the application of spectroscopy for structure validation and elucidation. The SpectraSchool Web site contains a variety of resource materials for students and teachers, designed to enhance the teaching and learning of spectroscopic and spectrometric methods (*36*). The resources include: interactive spectra which allow data to be compared for different compounds, video clips showing the practical aspects of instrumental techniques and self-assessment questions for students. The techniques covered are NMR (nuclear magnetic resonance), IR (infra red), MS (mass spectrometry) and UV-Vis (ultraviolet-visible). This project was funded by the Royal Society of Chemistry and is ideally positioned for future integration into ChemSpider.

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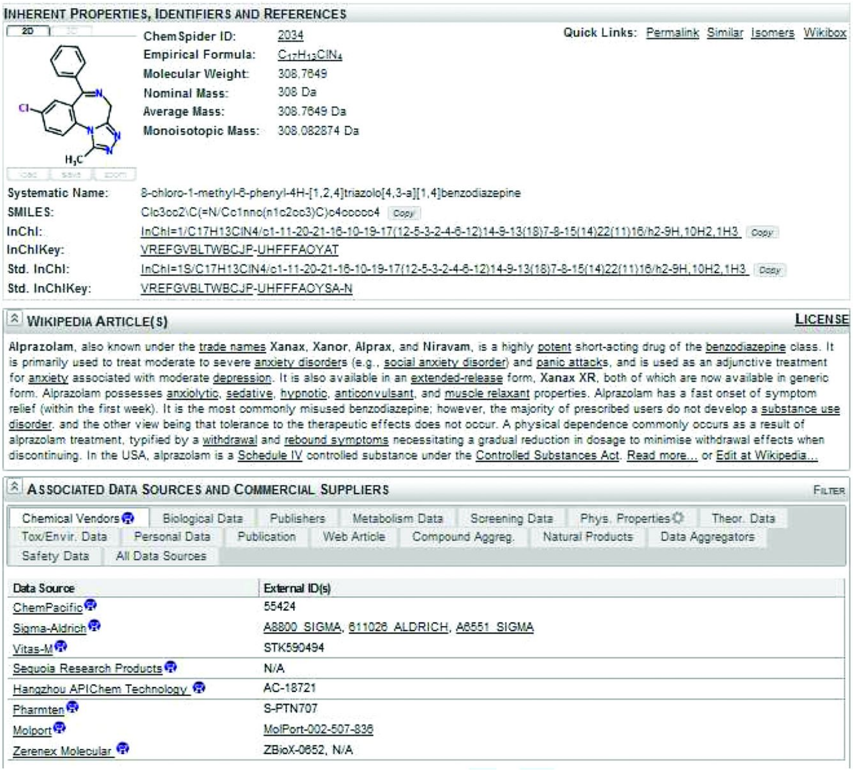

INHERENT PROPERTIES, IDENTIFIERS AND REFERENCES

Quick Links: Permalink Similar Isomers Wikibox

ChemSpider ID:	2034
Empirical Formula:	$C_{17}H_{13}ClN_4$
Molecular Weight:	308.7649
Nominal Mass:	308 Da
Average Mass:	308.7649 Da
Monoisotopic Mass:	308.082874 Da
Systematic Name:	8-chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine
SMILES:	Clc3cc2\C(=N/Cc1nnc(n1c2cc3)C)c4ccccc4
InChI:	InChI=1/C17H13ClN4/c1-11-20-21-16-10-19-17(12-5-3-2-4-6-12)14-9-13(18)7-8-15(14)22(11)16/h2-9H,10H2,1H3
InChIKey:	VREFGVBLTWBCJP-UHFFFAOYAT
Std. InChI:	InChI=1S/C17H13ClN4/c1-11-20-21-16-10-19-17(12-5-3-2-4-6-12)14-9-13(18)7-8-15(14)22(11)16/h2-9H,10H2,1H3
Std. InChIKey:	VREFGVBLTWBCJP-UHFFFAOYSA-N

WIKIPEDIA ARTICLE(S) LICENSE

Alprazolam, also known under the trade names **Xanax**, **Xanor**, **Alprax**, and **Niravam**, is a highly potent short-acting drug of the benzodiazepine class. It is primarily used to treat moderate to severe anxiety disorders (e.g., social anxiety disorder) and panic attacks, and is used as an adjunctive treatment for anxiety associated with moderate depression. It is also available in an extended-release form, **Xanax XR**, both of which are now available in generic form. Alprazolam possesses anxiolytic, sedative, hypnotic, anticonvulsant, and muscle relaxant properties. Alprazolam has a fast onset of symptom relief (within the first week). It is the most commonly misused benzodiazepine; however, the majority of prescribed users do not develop a substance use disorder. and the other view being that tolerance to the therapeutic effects does not occur. A physical dependence commonly occurs as a result of alprazolam treatment, typified by a withdrawal and rebound symptoms necessitating a gradual reduction in dosage to minimise withdrawal effects when discontinuing. In the USA, alprazolam is a Schedule IV controlled substance under the Controlled Substances Act. Read more... or Edit at Wikipedia...

ASSOCIATED DATA SOURCES AND COMMERCIAL SUPPLIERS

Data Source	External ID(s)
ChemPacific	55424
Sigma-Aldrich	A8800_SIGMA, 611026_ALDRICH, A6551_SIGMA
Vitas-M	STK590494
Sequoia Research Products	N/A
Hangzhou APIChem Technology	AC-18721
Pharmten	S-PTN707
Molport	MolPort-002-507-836
Zerenex Molecular	ZBioX-0652, N/A

Figure 1. A partial screen capture of the ChemSpider record following a search for "Xanax". The chemical record shows the structure, multiple identifiers, a snippet of the Wikipedia article and multiple links to Associated Data Sources and Commercial Suppliers as identified by the multiple tabs.

The Future of Online Chemistry Resources

The expansion in scope, capability and importance of the Internet as a source of information, data and contribution continues unabated. An increasing number of scientists will demand free and open access to literature, to patents, to data and to algorithms. The Open Source model for software that is now underpinning a growing digital culture will continue to flourish. As described by Anderson (*37*), the changing landscape of "Free" will lead to new business models within which new companies will succeed. Existing companies will need to reinvent themselves as participants within this changing industry or be left behind.

As smart phones become "genius phones" and iPhones morph to iPads there will be an increasing number of mobile computing applications which will only further increase accessibility to information. Access to all databases via a handheld device will be here (*38*). The promise of the Semantic Web will soon be fulfilled and as an increasing number of public databases become available semantic access to the data will be delivered soon after as resources such as ChemSpider mesh them into their services.

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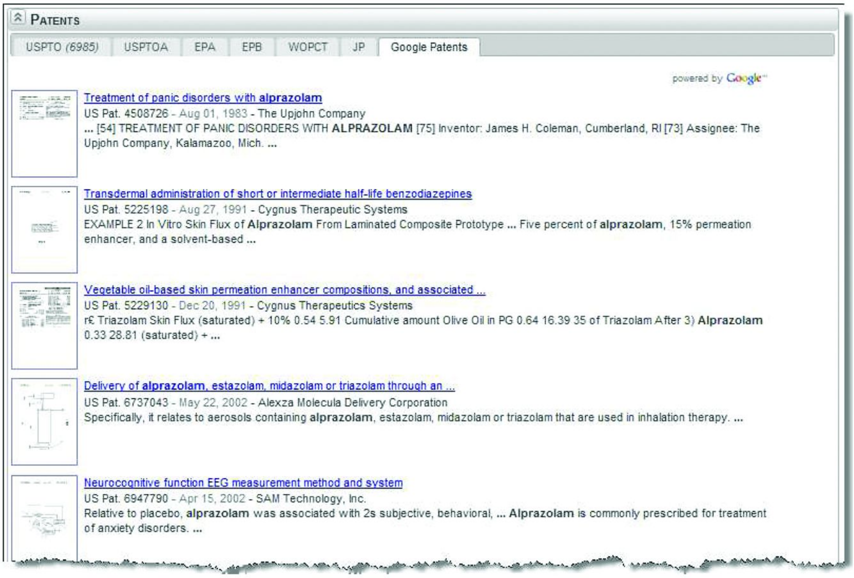


Treatment of panic disorders with alprazolam
US Pat. 4508726 - Aug 01, 1983 - The Upjohn Company
... [54] TREATMENT OF PANIC DISORDERS WITH **ALPRAZOLAM** [75] Inventor: James H. Coleman, Cumberland, RI [73] Assignee: The Upjohn Company, Kalamazoo, Mich. ...

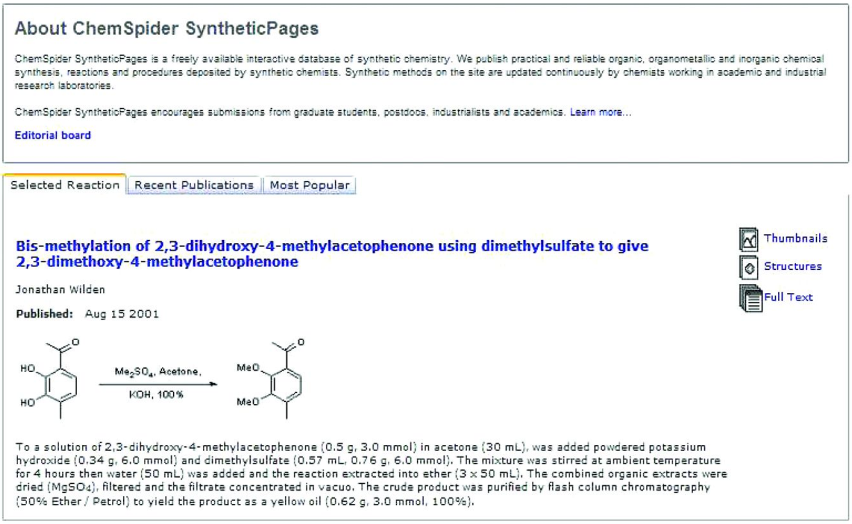
Transdermal administration of short or intermediate half-life benzodiazepines
US Pat. 5225198 - Aug 27, 1991 - Cygnus Therapeutic Systems
EXAMPLE 2 In Vitro Skin Flux of **Alprazolam** From Laminated Composite Prototype ... Five percent of **alprazolam**, 15% permeation enhancer, and a solvent-based ...

Vegetable oil-based skin permeation enhancer compositions, and associated ...
US Pat. 5229130 - Dec 20, 1991 - Cygnus Therapeutics Systems
r€ Triazolam Skin Flux (saturated) + 10% 0.54 5.91 Cumulative amount Olive Oil in PG 0.64 16.39 35 of Triazolam After 3) **Alprazolam** 0.33 28.81 (saturated) + ...

Delivery of alprazolam, estazolam, midazolam or triazolam through an ...
US Pat. 6737043 - May 22, 2002 - Alexza Molecula Delivery Corporation
Specifically, it relates to aerosols containing **alprazolam**, estazolam, midazolam or triazolam that are used in inhalation therapy. ...

Neurocognitive function EEG measurement method and system
US Pat. 6947790 - Apr 15, 2002 - SAM Technology, Inc.
Relative to placebo, **alprazolam** was associated with 2s subjective, behavioral, ... **Alprazolam** is commonly prescribed for treatment of anxiety disorders. ...

Figure 2. A partial set of hits from Google Patents displayed in ChemSpider following a search on Xanax.



About ChemSpider SyntheticPages

ChemSpider SyntheticPages is a freely available interactive database of synthetic chemistry. We publish practical and reliable organic, organometallic and inorganic chemical synthesis, reactions and procedures deposited by synthetic chemists. Synthetic methods on the site are updated continuously by chemists working in academic and industrial research laboratories.

ChemSpider SyntheticPages encourages submissions from graduate students, postdocs, industrialists and academics. Learn more...

Editorial board

Bis-methylation of 2,3-dihydroxy-4-methylacetophenone using dimethylsulfate to give 2,3-dimethoxy-4-methylacetophenone

Jonathan Wilden

Published: Aug 15 2001

To a solution of 2,3-dihydroxy-4-methylacetophenone (0.5 g, 3.0 mmol) in acetone (30 mL), was added powdered potassium hydroxide (0.34 g, 6.0 mmol) and dimethylsulfate (0.57 mL, 0.76 g, 6.0 mmol). The mixture was stirred at ambient temperature for 4 hours then water (50 mL) was added and the reaction extracted into ether (3 x 50 mL). The combined organic extracts were dried ($MgSO_4$), filtered and the filtrate concentrated in vacuo. The crude product was purified by flash column chromatography (50% Ether / Petrol) to yield the product as a yellow oil (0.62 g, 3.0 mmol, 100%).

Figure 3. A screenshot of the home page of ChemSpider SyntheticPages

ChemSpider will continue to grow in importance as one of the primary chemistry portals on the Internet. The number of compounds will continue to grow daily as additional publishers choose to participate in contributing to free structure-based discoverability by exposing their data. ChemSpider will expand from handling explicit chemical compounds to the support of compounds that cannot be represented by a specific connection table. As a result support

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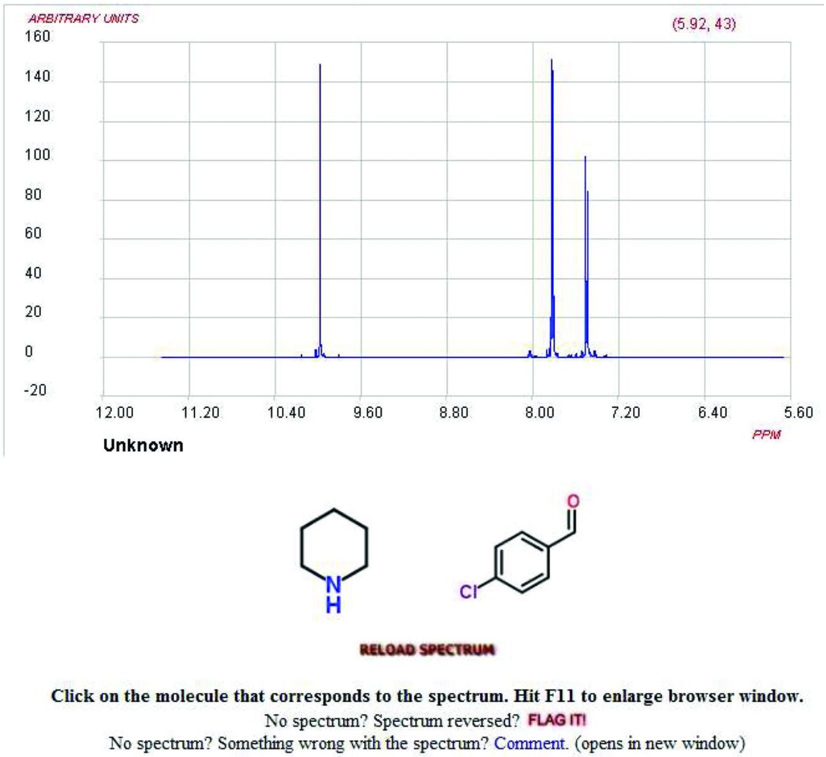

Click on the molecule that corresponds to the spectrum. Hit F11 to enlarge browser window.

No spectrum? Spectrum reversed? FLAG IT!

No spectrum? Something wrong with the spectrum? Comment. (opens in new window)

Figure 4. An early round of the spectral game showing a proton NMR spectrum and two possible chemical structures.

will improve for organometallics, polymers, minerals and other ambiguous compounds thus further expanding the coverage for this Internet portal for chemistry.

ChemSpider has recently undertaken a project entitled “ChemSpider Education” focused on delivering a subset of data and functionality for secondary school and undergraduate students studying chemistry. The majority of the *ca.* 25 million compounds on the ChemSpider database will bring little value to chemistry students early in their careers and much of the functionality delivered for mass spectrometrists and medicinal chemists will have little relevance. As a result, ChemSpider Education will deliver a selected slice of data and simplified interface to improve navigation and deliver capabilities tuned to the audience in question. Such a “personal” approach to delivering ChemSpider data slices will be repeated for multiple other user segments, including environmental scientists, toxicologists, and analytical scientists and so on. ChemSpider Education will continue the trend of utilizing game-based approach access to ChemSpider data in order to facilitate training, question and answer sets and so on. The intention is to encourage students to participate in the enhacement of the data on ChemSpider and to add their own content to the benefit of the entire community.

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Will Free Resources Disrupt Commerce?

The digital economy is a new economy. There are thousands of success stories born out of the innovations of the Internet. A number of organizations generate sizeable revenues from the creation of chemistry databases for the life sciences industry. Existing businesses generating revenues from chemistry databases likely perceive a risk from the increasing availability of free and open data available online for scientists and chem/bioinformaticians to mash-up into their in-house solutions. However, the primary advantage of commercial databases is that they have been manually curated addressing the tedious task of quality data-checking. The aggregation of data from multiple sources, both historical and modern, from multiple countries and languages and from sources not available electronically, offer greater coverage than what is available *via* an Internet search. However, how long will this remain an issue, and when will the data available electronically, for free, offer a sufficient return on investment to start to negatively impact the commercial chemical database suppliers?

Chemical Abstracts Service (*39*) and other commercial databases are certain to deliver significant benefit to its users for the foreseeable future, specifically to those users requiring structure-based patent searches to investigate intellectual property coverage. However, Internet queries are increasingly favored by scientists and the chemistry community is likely to reap increasing benefits from the growing number of free access services and content databases. Academics in particular are likely to have an increased focus on the use of free access databases. This will be further exaggerated in third-world countries where free access systems are the primary resources for information since commercial offerings have significant price barriers.

Librarians are retiring their print collections in favor of electronic repositories of chemical journals. Internet search engines are increasingly likely to be the first point of access for the majority of scientists for two simple reasons—they are fast and they are free. In terms of data quality issues, the Internet generation has already demonstrated a willingness to curate and enhance the quality of content as modeled by both Wikipedia and ChemSpider. With the improvements promised by the Semantic Web, if there are data of interest to be found, the search engines will facilitate it. As the President of CAS, Robert Massie, commented (*40*): "Chemical Abstracts has to be better than Google, better than our competitors, so that we can charge a premium price." This will become increasingly difficult and the redesign of commercial business models will be necessary. The timescale for this is up for discussion. Despite the rumored death knell for the classical business model of the science publishers, their business, for the time being, continues to grow unabated and successfully co-exist with the Open Access model. The same is likely to be true for the commercial and free chemistry databases.

Conclusion

Increasing access to free and open access databases of both chemistry and biological data is being encouraged by academics, funding agencies and pharmaceutical companies. Such databases will become more important in decision-making processes and attribution and assertion. The proliferation of freely-accessible data and information will need to be accompanied by approaches allowing data curation and validation to enable the development of qualified semantic platforms. Specifically, the development of a disambiguation dictionary mapping chemical identifiers to chemical compounds will likely provide one of the foundations of the semantic. As data-mining tools expand in their capabilities and performance, the chemistry databases available online now, and in the future, are likely to offer even greater opportunities to benefit the process of discovery.

The ChemSpider database has been online for just over three years. Initially developed on a shoestring budget and using a skeleton staff driven by passion and interest, it has already established itself as one of the premier chemistry sites on the Internet. Using a crowdsourced approach for data deposition, curation and validation ChemSpider has engaged the community to participate together for the common good as well as for the benefits of the individual. ChemSpider is already being used in teaching classes in chemical information retrieval (*41*) and is increasingly cited and utilized by educators. As a resource for students of chemistry ChemSpider already offers many advantages in terms of sourcing data and accessing information which just a few years ago would be locked behind a login to a commercial database via a library-hosted terminal. Now data are available for free, via any Internet-enabled device. As the Internet age of contribution continues these students will become critical participants in the development of the data bases serving them. The curation of data by students is already underway (*42*) and we believe that such contributions will continue expand. We live in exciting times.

About the Author

Antony Williams is the VP of Strategic Development and Host of ChemSpider at the Royal Society of Chemistry. He has spent over a decade in the commercial scientific software business as Chief Science Officer for Advanced Chemistry Development. He was trained as an NMR spectroscopist by training and has (co-)authored over 100 peer-reviewed publications and multiple review articles and book chapters. He continues to focus his passion for providing access to chemistry-related information to the masses with the RSC-ChemSpider team and innovate novel approaches for improved access to chemical data online. He can be contacted at antony.williams@chemspider.com.

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of new structures from Prospected RSC articles, as well as a growing number of integration projects, sits squarely on the shoulders of Aileen Day. Thank you! The ChemSpider support team of Jan Davies and David Sharpe provide daily support to our users. The ChemSpider project continues to expand in breadth and impact with the support of David James and Richard Kidd.

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Chapter 3

Using Semantically-Enabled Components for Social Web-Based Scientific Collaborations

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The article reviews how various publishing and social networking components on the Web might be semantically enabled to create an environment in which connections between diverse subjects, both within a given domain such as chemistry, and across domains, can be facilitated. An example is constructed called SemanticEye, and illustrated using vocabularies based on FOAF (Friend of a Friend), together with DOI and InChI identifiers.

1. Connecting the Sciences

Modern science is characterised by ever increasing and overlapping boundaries, both within sub-domains and venturing into newly emerging disciplines. To quote Ted Nelson (*1*), “Everything is deeply inter-twingled. In an important sense there are no subjects at all; there is only all knowledge, since the cross-connections among the myriad topics of this world simply cannot be divided up neatly”. A typical modern academic chemistry department for example may in fact both actively teach and research on topics representing much of the diversity found in science, technology and medicine, and even extending to the creative arts and design. In this chapter, we will explore how some of the new Web-based technologies might be able to facilitate individuals to make new connections across this diversity, in order to increase their holistic view of science and widen contacts with potential new collaborators.

Faced with the seemingly overwhelming complexity and diffuseness of a topic, the natural starting point for most people is understandably to focus on identifying other people or groups who with their own acquired expertise may provide a focal point for exploration. Many scientific collaborations still

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traditionally begin face-to-face (*2*) with the initial contact made primarily by networking at lectures, seminars, conferences and meetings. Enjoyable though such occasions may be, they provide only a partial coverage of all potential collaborators. What then is needed to help broaden the pool? The Internet nowadays is an obvious place to start, and we suspect that many people reading this article would be able to cite instances of collaborative success involving participants whom they only know through utilizing the classical Web mechanisms, including search engines, email and perhaps telephone contacts. The serendipitous nature of such connections can however seem frighteningly random, and we must all wonder how many connections are simply missed because of the lack of any more systematic way in which to initialise them. A typical (and because people are involved, inevitably autobiographical) example of one such serendipitous contact is described here, if only to illustrate the challenging nature of the connections between diverse and many disciplines that must be made. In what follows many semi-technical terms and individuals are highlighted, each of which have their own semantic meaning, connections and context! Some of these terms are italicised below (the selection is to some extent arbitrary) to help emphasise concepts introduced later in this article. Many of the connections described below have found their way into taught lectures, and indeed articles such as this one.

In 1978, one of the present authors was asked to teach an undergraduate course on *pericyclic reactions*, which in fact he still does to this day! This is an area of *organic chemistry* that combines the *taxonomy* of a particular class of reactions proceeding via *cyclic transition states*, with the requirement of a deeper theoretical analysis based on *symmetry* and *group theory* (a topic in *mathematics* which goes back to 1832 and the remarkable individual Evariste Galois (*3*)) and an application of *quantum mechanics* known as *molecular orbital theory*. A new pedagogic approach was sought which could be used to combine some degree of rigor with the clarity that can be achieved without overwhelming mathematical content. The aspect of *transition state aromaticity* was settled upon (*4*), which built on very imaginative connections to *molecular orbital theory* made by first *Heilbronner* and then *Zimmerman* (*5*). This managed to inter-twingle the diverse topics of *topology*, introduced in 1847 by *Listing* (*6*) and exemplified by half-twisted *Möbius* bands, *Galois*' *group theory*, a theoretical analysis of *aromaticity* formulated by *Huckel* in 1931 (*7*) and the application of this property to cyclic transition states (*8*), leading to the concept of *Möbius aromatic transition states*. One consequence of focusing on these connections was that some simple logical inferences suggested themselves. The first was that *Möbius aromaticity* might not be restricted to *transition states*, but should also manifest in stable *molecules*. This hope has in fact been spectacularly vindicated in the last few years, with many such systems having now been discovered. As a result, the topic is now regarded as mainstream chemistry (*9*).

The second was the inference that the *Möbius* band was in fact just one of a family of twisted topological objects, connected to another area of mathematics known as *knots* and *manifolds* (made famous by the *Poincare conjecture* (*10*)). This can be more pithily expressed by the question (first asked in 2005 (*11*)) "can stable aromatic molecules exhibiting topologies with more than one half twist exist"?. The answer soon turned out to be yes (*12*), but this merely led to the next question of "why"? The answer it turned out was well known to both *molecular biologists* (*13*) and mathematicians (*14*), who knew it as the topological property of *writhe*. Chemists were not so familiar with *writhe*, largely because the previously applied contexts of *DNA oligomers* and *topoisomerase enzymes* was too far removed from *small molecules* for the connection to have been prominently made. It took a building fire alarm to enforce a conversational proximity with a physical chemist working on *DNA*, whose lecture on the very topic had just been interrupted and who therefore fortuitously had the appropriate conceptual diagrams immediately to hand! Formalizing the connection still required one further stroke of luck. An email, normally only circulated within a small group but on this occasion finding its way to a wider departmental list, advertised an imminent seminar on the knotting propensity of *polymer chains* to be delivered by a visiting physicist from Israel. Although there was no mention of *writhe* in the title of the talk, speculative attendance at the seminar anyway revealed (but only during question time at the end) that the student whose work had just been described had also written computer code for numerical evaluation of this property. A number of mail and telephone exchanges were still required for both parties to normalise their interpretations of each other's terminologies and definitions (including the loss of a mysterious factor of two, due to the implicit semantics each had assumed). The final outcome (*15*) represents an interesting fusion of concepts from quite different areas of chemistry and mathematics, by two authors who have in fact never met physically. The story should perhaps end with one more unexpected connection, this time between two different areas of chemistry. A report had recently appeared (*16*) which claimed the isolation of a molecular *metallacycle* containing a band of 15 *manganese* atoms, and which appeared to sustain as many as six half twists in the cycle. However, the authors' published analysis of the twisting revealed a discrepancy which, lacking any clear explanation, had been relegated to a puzzled footnote in their article. Quantifying the contribution of *writhe* provided a full resolution of that discrepancy (*17*).

We can see in the preceding story both the diversity of modern science and chemistry, but also how fragile the social mechanisms were that enabled the correct concepts and connections to be identified by various pairs or groups of individuals. Lectures, seminars, and indeed fire-alarms all played a crucial role, not to mention a modicum of luck! It should also be noted that the chronology described above occurred over a period of some thirty years, and in a manner punctuated by many fits and starts whilst the catalysing connections were made. It is this very duration and often accidental aspect that has led us to ask whether procedures might be constructed that can reduce our dependence on luck, and provide a more systematic and accelerated way of initiating scientific connections together with the appropriate collaborations. Indeed, Kurzweil in his futuristic exploration (*18*) envisages the coming together of humans and machine as leading to a singularity in human evolution. The scope of this article is rather less apocalyptic; the intention is to explore several mechanisms facilitating what has become known as the process of semantic discovery, and how this might start to impact upon how a subject such as chemistry is both taught and researched. It is not our intention in this article to provide a comprehensive review of all the

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mechanisms being explored for semantic enablement of chemical information and knowledge, although this theme is also taken up in other articles in this book.

2. Semantic Enablement of Social Networking as a More Effective Resource for Collaboration

2.1. Inadequacies of Web 2.0 for Establishing Collaborations

Web 2.0 applications essentially facilitate interactive information sharing and collaboration on the Internet. In contrast to traditional Web sites where users are passive information consumers, a Web 2.0 site allows its users to contribute to the Web site's content. Web 2.0 sites currently serve as an Internet mechanism for establishing contacts between potential collaborators, and for individuals to try to establish semantic connections (inter-twingling to use Nelson's term) between ideas. Despite the opportunities, the concept still has major shortcomings which could deter scientists. In particular, many such sites tend to be what are referred to as information silos. Users entering them must manually maintain a separate personal profile for each site, and most are designed to be accessed by humans *via* Web browsers. Absent from many of these sites are semantic data, metadata and interfaces which would enable the participation of software agents that could perform useful functions such as connecting users who have common interests, but who are not necessarily members of the same social network. Indeed such a notion might run counter to prevailing business models of Web 2.0 social networks whereby users along with the content they create are essentially ring fenced. In the case of finding collaborators, no single social network provides a broad enough pool to be a serious alternative to locating collaborators at *e.g.* highly focused scientific conferences. As will be discussed later, what has become known as Web 3.0 technologies may have the potential for rectifying these shortcomings and thereby creating new opportunities for chemical innovation and discovery.

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3. Web 3.0 and the Semantic Web

The next generation of global information system, colloquially known as Web 3.0, adopts the Semantic Web approach to content discovery. The Semantic Web is an established framework for the navigation and discovery of information assets and services on the Web. Unlike Web 2.0 interfaces, which require human participation for information dissemination, the Semantic Web also permits the participation of software agents to assist with the dissemination. Agents are not expected to predict semantic meaning from existing Web content using clever algorithms. Instead, content owners invest some effort in lacing the content with appropriate metadata, with the payback being that more readers and agents would be able to locate the content and understand it.

The Semantic Web is expressed in a formal specification called the Resource Description Framework (RDF) (*19*), a vocabulary for constructing relationships based on triples. An RDF triple describes how a *subject* Web resource relates to an *object* Web resource via a *predicate* attribute. The *object* resource can, in turn, be the *subject* resource in another triple, thereby building up a semantic map with the potential to grow *ad infinitum*. RDF triples are reconciled either in N-Triple notation, which applications normally read to construct the semantic map, or in XML. Names are prefixed by namespaces to ensure their uniqueness. The RDF Schema defines the data specific to an RDF vocabulary normally for a given knowledge domain. Knowledge domains can be combined by simply combining RDF Schemas.

The following sections present technologies prototyped both at Imperial College and externally, and which we think might potentially influence the evolution of Web 3.0 in a manner that we think may benefit future collaborative scientific research.

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3.1. Semantic-Enhancement of Journal Articles: SemanticEye

SemanticEye (*20*) was developed in 2006 as a lightweight ontology and implementation for supporting Semantic Web technologies for chemical electronic publishing metadata. Its purpose is to facilitate the detection of (perhaps unexpected) connections between different articles in a collection. The relationships between articles are established by common authors and/or common molecules, the latter represented as IUPAC International Chemical Identifiers (InChI). The InChI was developed to provide a standard human readable way to encode molecular information and to facilitate the Web based searching of the same. The InChI expresses molecular information by taking a layered approach where each successive layer adds additional detail to the identifier. The layers are formula, connectivity (excluding formal bond orders), isotopes, stereochemistry and tautomers (on or off). Charges are not part of the InChI layers but are appended to the end of the InChI string. The specific layers are generated automatically from the structures and depend on the structural detail provided. The reconciliation of the InChI for searching has been discussed in detail (*21*).

Each article in SemanticEye contains at least one author and one InChI. SemanticEye makes no assumption and enforces no restriction on the level of detail that an InChI can have. If an InChI for a structure in Article A has more detail than an InChI for the same structure in Article B, Article B would currently not link to Article A. Because of the layered approach of the InChI, a facility (or Semantic Web agent) for linking up InChIs at lower layers of detail should in theory be straightforward to implement. The ontology also includes each article's Document Object Identifier (DOI) to enable aggregation, *via* the DOI, with established bibliographic ontologies such as BIBO (*22*)

XMP (*23*), an RDF syntax designed by Adobe for the management and storage of documents, is at the core of SemanticEye's architecture. As with music files, XMP is embedded in a document and travels with the document when its location changes. Documents can be in any format, and Adobe has published a specification for embedding XMP in some of the most common including HTML, Word, SVG, JPEG, TIFF, GIF, and PDF. Adobe's successes with propelling file formats, particularly PDF and SVG (*24*), into global *de facto* standards hints towards the long term viability of XMP, provided of course that it is made straightforward to use and reuse. Adobe supports XMP editing within its software suite; an API is also supported.

The uptake of XMP by scientific publishers was initially very limited due to the slow growth of RDF as a whole. Moreover, only a succinct specification, which includes the Dublin Core RDF Schema, is handled by Adobe software. Most XMP implementers would want to extend the vocabulary with their own RDF Schemas or external Schemas. A significant example is the Publishing Requirements for Industry Standard Metadata (PRISM) XMP (*25*) which was implemented to allow PRISM metadata to be embedded in multimedia objects accessible online.

XMP expects its RDF serialised in XML and does not support any of the other RDF representations. In contrast to the many possible ways of representing an RDF/XML vocabulary (known as RDF polymorphism), XMP extensions require a documented (*26*) restrictive RDF serialisation to enable the correct handling by Adobe software. If XMP employed an appropriate ontology in the Web Ontology Language, or OWL, such restrictions could be formally defined.

Caveats notwithstanding, XMP is now starting to gain traction amongst scientific publishers. Elsevier started embedding their articles with XMP in 2007 and their use of XMP has been evolving based on experience (*27*). Nature Publishing has implemented a workflow solution to handle XMP capture whereby automated batch-processing extracts information from XML files and outputs standardized validated PDF files with the XMP embedded. All Nature articles published since December 2008 now contain XMP (*28*).

XMP is also supported by popular citation-management programs. Both Zotero (*29*) and Mendeley (*30*) read embedded XMP metadata from PDFs if available. However, neither of them populate PDF documents with XMP metadata if the documents do not initially have them.

XMP capture can also be achieved manually by inputting metadata using a form tool (Figure 1), which is a feature in several Adobe products including Acrobat Professional. For capturing user defined metadata, the form tool can be enhanced by editing a panel description file. Alternatively, XMP can be edited outside of the software and imported, an approach which can potentially be automated using chemical data capture techniques. Sustainable metadata capture processes would normally require multiple interoperable software tools. The importance of open standards such as XML for software interoperability is exemplified in an Open XML architecture proof of concept (*31*).

To improve RDF navigation, XMP metadata are repurposed into a simplified RDF ontology (Figure 2) and managed centrally in an RDF repository called Sesame. There are two classes of RDF repositories, native triple stores and relational databases. Native triple stores, such as Virtuoso or AllegroGraph are built from the ground up and optimised for archiving RDF triples. Relational databases utilise establish products such as Oracle or mySQL, and software, such as Sesame or Jena, map the RDF schema to a relational schema.

So far, publishers have been reluctant to implement Semantic Web models such as Semantic Eye, presumably because the business value is not clear enough. Because the business value of an application can be improved if it is "inter-twingled" with other applications, we also investigated how SemanticEye can be integrated into Social Networks.

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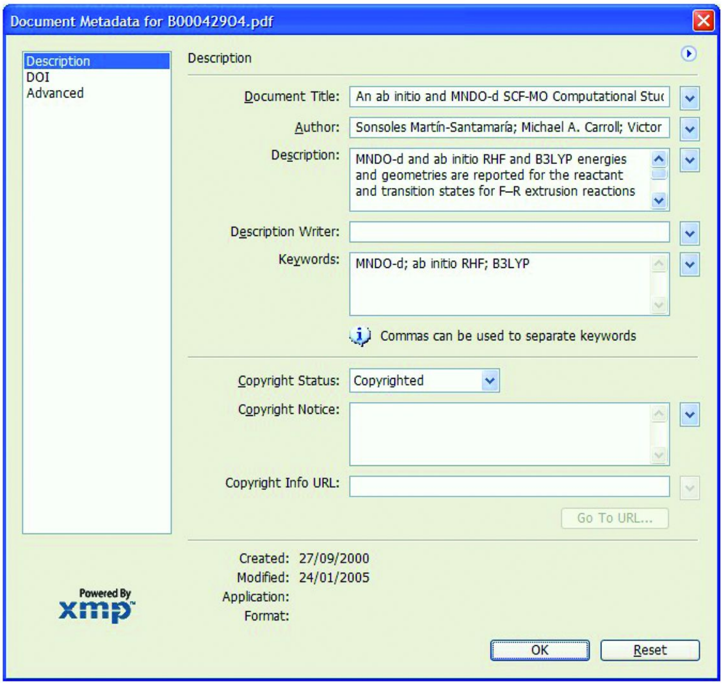
Document Metadata for B00042904.pdf
Description
DOI
Advanced
Description
Commas can be used to separate keywords
Go To URL...
Powered By xmp
OK
Reset

Document Title: An ab initio and MNDO-d SCF-MO Computational Stu(

Author: Sonsoles Martín-Santamaría; Michael A. Carroll; Victor

Description: MNDO-d and ab initio RHF and B3LYP energies and geometries are reported for the reactant and transition states for F–R extrusion reactions

Description Writer:

Keywords: MNDO-d; ab initio RHF; B3LYP

Copyright Status: Copyrighted

Copyright Notice:

Copyright Info URL:

Created: 27/09/2000

Modified: 24/01/2005

Application:

Format:

Figure 1. Acrobat Professional XMP Tool

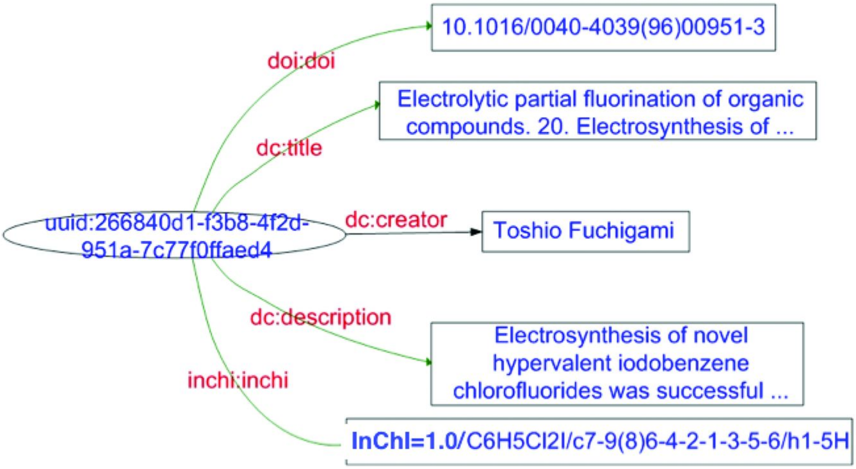
uuid:266840d1-f3b8-4f2d-951a-7c77f0ffaed4
doi:doi
10.1016/0040-4039(96)00951-3
dc:title
Electrolytic partial fluorination of organic compounds. 20. Electrosynthesis of ...
dc:creator
Toshio Fuchigami
dc:description
Electrosynthesis of novel hypervalent iodobenzene chlorofluorides was successful ...
inchi:inchi
InChI=1.0/C6H5Cl2I/c7-9(8)6-4-2-1-3-5-6/h1-5H

Figure 2. SemanticEye triples for a single journal article

4. FOAF (Friends of a Friend): A Semantic Web Vocabulary for Social Networks

4.1. FOAF Overview

FOAF is essentially an RDF vocabulary of terms for constructing machine readable profiles used in home pages and social networks. It allows the semantic expression of "friends", publications, public collaborations and other activities. Its architecture is decentralised; FOAFs are expected to be maintained within home pages, not in centralised databases. An example of a personal FOAF is given in Figure 3.

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```
<foaf:Person>
 <foaf:name>Omer Casher</foaf:name>
 <foaf:mbox_sha1sum>0cd8fa86a146f025e635ad43f64537ecdc7fd408
 </foaf:mbox_sha1sum>
 <foaf:workplaceHomepage rdf:resource="www.gsk.com"/>
 <foaf:homepage rdf:resource="http://www.omercasher.com/"/>
 <foaf:knows>
 <foaf:Person>
 <foaf:name>Henry Rzepa</foaf:name>
 <foaf:mbox_sha1sum>0d26f3beb220c20f1fced27930005e5f0d0d23c2
 </foaf:mbox_sha1sum>
 <foaf:homepage rdf:resource="http://www.ch.ic.ac.uk/rzepa/"/>
 <foaf:workplaceHomepage rdf:resource="http://www.ic.ac.uk/"/>
 </foaf:Person>
 </foaf:knows>
….
</foaf:Person>
```

Figure 3. Example of a Personal FOAF

```
<foaf:Group>
 <foaf:name>Blue Obelisk</foaf:name>
 <foaf:member>
 <foaf:Person>
 <foaf:name>Henry Rzepa</foaf:name>
 <foaf:homepage rdf:resource="http://www.ch.ic.ac.uk/rzepa/"/>
 <foaf:workplaceHomepage rdf:resource="http://www.ic.ac.uk/"/>
 </foaf:Person>
 </foaf:member>
<foaf:member>
 <foaf:Person>
 <foaf:name>Egon Willighagen</foaf:name>
 <foaf:homepage rdf:resource="http://chem-bla-ics.blogspot.com/"/>
 </foaf:Person>
 </foaf:member>
….
</foaf:Group>
```

Figure 4. Example of a group FOAF

The FOAF RDF vocabulary is expressive enough to allow for the creation of rich scientific profiles that, within a social network setting, can lead to "research serendipity". However, the uptake of FOAF has been slow in chemistry presumably because maintaining personal FOAFs is time consuming and the value to scientists has not been effectively demonstrated. We feel that a widespread adoption of this or similar vocabularies among chemists will only be achieved if it is driven by influential organisations, namely the publishers.

Nevertheless, some grass roots adoption has been taking place, one example being the Blue Obelisk organisation (http://www.blueobelisk.org/) that maintains a group FOAF of its members (Figure 4). Better FOAF software tools, particularly those that understand chemical semantics, are needed.

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4.2. FOAF Aggregation

FOAF aggregation is essentially a process which combines multiple FOAFs to create broadened profiles, without the need for manual editing. FOAF aggregation is attractive for communities where devolved control is required. However, using an individual's personal information outside of the individual's control has sociological issues. FOAF aggregations therefore need to be handled appropriately. Because the goal of this investigation is primarily to add value to scientific collaborations, FOAF aggregations are restricted to the machine assisted establishment of scientific collaborations within social networks. The following sections describe how this is achieved.

4.3. FOAF Aggregation with SPARQL

4.3.1. The SPARQL Query Standard

SPARQL is both a data access protocol and an RDF query language. Ratified in January 2008 and widely supported by RDF repositories, it is the *de facto* RDF query standard replacing a multitude of legacy query formats. SPARQL can be used to query diverse sources where the RDF data is either native or dynamically generated. The query results can either be hit lists or, more elaborately, RDF constructions. Hence one or more SPARQL queries across multiple RDF sources can generate useful aggregations as RDF, a prime example being FOAF aggregations.

Using a suitable SPARQL query, SemanticEye would be able to output all of an author's collaborators as FOAF "friends" which can then be easily added to the author's personal FOAFs. Alternatively, SemanticEye can output, as a FOAF group, all of the scientists associated with a common InChI identifier. No manual editing of these outputs is needed.

FOAF aggregations could feed into any social network which understands FOAF. However, most mainstream social networks do not support FOAF, the one noteworthy exception being LiveJournal (*32*).

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4.3.2. Using SPARQL Queries To Identify Scientists Working on the Same Molecules

Auto-generated SemanticEye FOAFs enable all scientists who actively publish to have up-to-date scientific profiles, the values of which can potentially be improved by aggregation with FOAF outputs from a variety of sources. The following sections illustrate the creation of such an aggregation of multiple FOAFs for a single person with the help of SPARQL.

4.3.3. Identifying a Scientist's Existing Collaborators in FOAF

SemanticEye is queried for all co-authors associated with any articles having "rzepa" as one of its authors (Figure 5). The SPARQL CONSTRUCT feature is used to output the RDF triples serialised as FOAF.

```
PREFIX dc: <http://purl.org/dc/elements/1.1/>
PREFIX foaf: <http://xmlns.com/foaf/0.1/>

CONSTRUCT {
<http://www.ch.ic.ac.uk/people/rzepa> foaf:knows _:v2 .
_:v2 <http://www.w3.org/1999/02/22-rdf-syntax-ns#type> foaf:Person .
_:v2 foaf:name ?creator .
}
WHERE
{
 ?document1 dc:creator ?author .
 FILTER regex(?author, "rzepa", "i") .
 ?document2 dc:creator ?creator .
 FILTER (?document2 = ?document1 && !regex(?creator, "rzepa", "i") )
}
```

Figure 5. SPARQL Query on SemanticEye Triples to identify scientific collaborators

```
PREFIX dc: <http://purl.org/dc/elements/1.1/>
PREFIX inchi: <http://www.inchi.org/1.12/>
CONSTRUCT {
 <http://rdf.openmolecules.net/> <http://www.inchi.org/1.12/inchi>
?inchi .
}
WHERE
{
 ?document1 inchi:inchi ?inchi .
 ?document1 dc:creator ?author .
 FILTER regex(?author, "rzepa", "i") .
}
```

Figure 6. SPARQL Query on SemanticEye Triples to identify molecules of interest

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4.3.4. Aggregating the FOAF To Include the Scientist's Molecules of Interest

SemanticEye is queried for the InChI metadata associated with any articles having “rzepa” as one of its authors (Figure 6) and a FOAF is outputted as RDF triples. The InChI namespace used here is “http://www.inchi.org/1.12/” and it is given the alias “inchi”. The output is then aggregated with the FOAF containing scientific collaborators, as presented in the previous section, by a simple concatenation of the two RDF triple outputs. The FOAF aggregation is illustrated as XML in Figure 7.

```
 <foaf:Person>
  <foaf:name>Henry S. Rzepa</foaf:name>
  <foaf:knows>
  <foaf:Person>
  <foaf:name>Dave Widdowson</foaf:name>
  </foaf:Person>
  </foaf:knows>
  <foaf:interest>
  <rdf:Description rdf:about=" http://rdf.openmolecules.net"
rdfs:label="Molecule">
  <inchi:inchi>INChI=1/C6H12O2/c1-2-4-8-6-5-7-3-1/h1-6H2</inchi:inchi>
  <inchi:inchi>INChI=1/C21H17ClN4O3/c1-12-23-20-21(29-12)26(14(3)28)24-
19(15-7-5-4-6-8-15)17-11-16(22)9-10-18(17)25(20)13(2)27/h1-3H3,4-
11H/b24-19-</inchi:inchi>
  </rdf:Description>
  </foaf:interest>
  <foaf:publications>
  <foaf:Document rdf:about="http://dx.doi.org/10.1039/b000429o"
rdfs:label="Journal">
  <dc:title>An ab initio and MNDO-d SCF-MO Computational Study of
Extrusion Reactions of R2I-F Iodine (III) via Dimeric, Trimer and
Tetrameric Transition States</dc:title>
  </foaf:Document>
  </foaf:publications>
  </foaf:Person>
```

Figure 7. Personal FOAF of SemanticEye output

```
PREFIX dc: <http://purl.org/dc/elements/1.1/>
PREFIX foaf: <http://xmlns.com/foaf/0.1/>
PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
PREFIX inchi: <http://www.inchi.org/1.12/>

CONSTRUCT { <http://www.inchi.org/1.12/inchimolecule> rdf:type
foaf:Group .
<http://www.inchi.org/1.12/inchimolecule> foaf:member _:v1 .
_:v1 rdf:type foaf:Person .
_:v1 foaf:name ?creator .
}
WHERE
{
 { ?document inchi:inchi ?inchi .
 ?document dc:creator ?creator .
 FILTER regex(?inchi, "INChI=1/C6H5Cl2I/c7-9", "i") . }
}
```

Figure 8. SPARQL Query on SemanticEye Triples to group authors according to a molecule of interest

```
<foaf:Group>
<foaf:member>
 <foaf:Person>
 <foaf:name>David Wiedenfeld</foaf:name>
 </foaf:Person>
 </foaf:member>
 <foaf:member>
 <foaf:Person>
 <foaf:name>Rashmi Pundeer</foaf:name>
 </foaf:Person>
 </foaf:member>
....
</foaf:Group>
```

Figure 9. Group FOAF of SemanticEye output

4.3.5. Grouping Authors by a Molecule of Interest

SemanticEye is queried for all journal authors associated with an InChI molecule of interest (Figure 8) and outputs a FOAF Group of the authors (Figure 9).

4.3.6. Creation of a Scientific Profile by Aggregating FOAFs from Multiple Sources

This section illustrates how an individual's scientific profile can be built up automatically by aggregating SemanticEye FOAF outputs with those from other resources, in this case ChemSem and the Imperial College Professional Web Pages. ChemSem (*33*) is a seminar notification system, which includes the CML XML vocabulary, and was built using open source software. It outputs an RDF site summary (RSS 1.0) feed which can potentially "inter-twingle" with other RSS feeds based on common metadata, and which provides information about individuals giving seminars at the institute. Another source of personal information comes from the Professional Web Page (PWP) database, with the content of this database such as publication lists populated automatically using technology provided by Symplectic (*34*). Using an XML schema definition (XSD) and an XML stylesheet transform (XSLT), the database can output a personalised FOAF for each academic.

The FOAF aggregation from the three resources for Henry S. Rzepa is illustrated in Figure 10.

5. The Current Status of Online Resources, Social Networking, and Digital Libraries

In the previous sections, the automated creation of a scientific profile was demonstrated. Such a profile is invaluable for improving a scientist's coveted visibility via a "Web presence" and, in turn, their chances of establishing new collaborations. A good Web presence, can be established, at a minimum, by

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a well-populated and up to date list of publications together with a home page describing current research and areas of expertise. Aggregated FOAFs fit well here and can be incorporated now with minimal effort.

The Web however provides additional channels for improving visibility that are particularly advantageous for up-and-coming scientists without a well-known research portfolio and publication list. A good idea, irrespective of the status of its source can easily be brought to the attention of others on the Web and a community can be formed. Such communities, which enable like-minded people to meet, are often underpinned by Web 2.0 technologies.

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5.1. The Relevance of Some Existing Web 2.0 Technologies

There is a prevailing notion that the Semantic Web and Web 2.0 are competing technologies. We feel that the two are actually complementary and should really be exploiting each other's strengths. Indeed some Web 2.0 technologies are beginning to link in to the Semantic Web by various means. Hence, the Semantic Web technologies discussed in this paper can start to be realised now if incorporated within Web 2.0 applications that understand RDF. The following sections discuss Web 2.0 technologies and cite several examples.

```
<foaf:Person>
 <foaf:name>Henry S. Rzepa</foaf:name>
 <foaf:title>Professor</foaf:title>
 <foaf:knows>
 <foaf:Person>
 <foaf:name>Dave Widdowson</foaf:name>
 </foaf:Person>
 </foaf:knows>
 <foaf:interest>
 <rdf:Description rdf:about="http://rdf.openmolecules.net/"
      rdfs:label="Molecule">
 <inchi:inchi>INChI=1/C6H12O2/c1-2-4-8-6-5-7-3-1/h1-6H2</inchi:inchi>
 <inchi:inchi>INChI=1/C21H17ClN4O3/c1-12-23-20-21(29-12)26(14(3)28)24-19(15-7-5-
      4-6-8-15)17-11-16(22)9-10-18(17)25(20)13(2)27/h1-3H3,4-11H/b24-19-
      </inchi:inchi>
 <inchi:inchi>INChI=1/C18H28/c1-2-4-6-8-10-12-14-16-18-17-15-13-11-9-7-5-3-1/h1-
      2,7,9-10,12,17-18H,3-6,8,11,13-16H2/b2-1-,9-7-,12-10-,18-17-</inchi:inchi>
 </rdf:Description>
 </foaf:interest>
 <foaf:publications>
 <foaf:Document rdf:about="http://dx.doi.org/10.1039/b000429o"
      rdfs:label="Journal">
 <dc:title>An ab initio and MNDO-d SCF-MO Computational Study of Extrusion
      Reactions of R2I-F Iodine (III) via Dimeric, Trimer and Tetrameric
      Transition States</dc:title>
 </foaf:Document>
 </foaf:publications>
 <foaf:publications>
 <foaf:Document
      rdf:about="http://www.ch.ic.ac.uk/pss/index.php?page=view&amp;action=view&a
      mp;ID=633" rdfs:label="Seminar">
 <dc:title>Organic Computational chemistry, lecture 1</dc:title>
 <dc:description>An introduction to molecular modelling, scope of lecture, basic
      definitions and scales of molecular models</dc:description>
 </foaf:Document>
 </foaf:publications>
```

Figure 10. Example FOAF Aggregation of a single person from 3 sources: SemanticEye (blue, lines 1−19), ChemSem (orange, lines 20−27), Professional Web Page (green, lines 28−36). (see color insert)

5.1.1. Blogs

Blogs (from: "Web log") are user-created Web sites, usually maintained by an individual, with regular entries of commentary, descriptions of events, or other material such as graphics or video. Entries are commonly displayed in reverse-chronological order. Many blogs provide commentary or news on a particular subject, whilst others function as more personal online diaries. A typical blog combines text, images, and links to related resources. The open interactivity of comments is an important feature. Something of a new medium, the purpose of a blog is still being actively explored by its proponents.

Several blogs are noted here to illustrate the diversity of approaches. The totally synthetic blog (*35*) came to substantial prominence by highlighting a report in a noteworthy journal (*36*) describing the use of sodium hydride as an oxidant. Within days, a community had coalesced around discussion of the scientific issues raised in the article, and the eventual outcome was its formal withdrawal. The blog posting highlighted the problems faced with the modern refereeing processes, and is notable for the speed of events catalysed by its posting. Another blog (*37*) has come to the fore for its crusading approach to many important problems and issues facing scientific publishing. Significantly, it reaches many communities that conventional chemistry journal publishing does not. Other blogs address a more conventional chemistry audience. One with a wide readership (*38*) highlights, often with critical comment, recent interesting publications in computational chemistry; many journals also now offer a similar service for their own readership. To be cynical, in highly interconnected world, “The only thing worse than being talked about is not being talked about” (*39*) and it is no longer considered sufficient to merely publish a new scientific result, one must also strive to get it discussed, and perchance “inter-twingled”, as widely as possible. Another blog provided by one of the present authors (*40*) was set up to disseminate original observations and molecular modelling computations deriving from (*inter alia*) materials prepared during the course of undergraduate lectures and tutorials. This type of material often has no outlet in conventional scientific journals and books, and would otherwise be lost to science.

“Blogging” is thus seen as a relatively effortless way to connect with like-minded people, to improve visibility and become part of a community. Blogs are also a particularly useful way to share interesting or perhaps even constructively critical findings that would otherwise not be published. They are also very effectively and rapidly (within minutes of being posted) indexed by search engines such as Google, although not (as yet) by conventional agencies such as Chemical Abstracts.

5.1.1.1. Semantic Blogs

Several exemplars of semantically enabled blogging have been reported with one of the earliest coming out of HP Labs (*41*). A relatively recent semantically enabled blog was in fact set up (*40*) by one of the present authors (*42*). This makes use of tools such as Zemanta (*43*) for creating in-text Web hyperlinks that

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integrate to important “Linked Open Data” resources like DBpedia (*44*), and it also includes an automatic tagging service (*45*) to detect and highlight common terms, expressing them as RDF metadata declarations within the blog itself. The detected terms themselves however contain no overtly chemical meanings, and it would be desirable to link such a service to chemical and molecular ontologies.

5.1.2. Wikis

A Wiki is a collaborative Web site where content is created and maintained by multiple authors using a simple online editor. This concept is sometimes described as write-many-read many, and is thus distinct from a blog which tends to be associated with an individual. The best-known example is of course Wikipedia, within which the chemical content is now impressively large. Access to a Wiki can be either open or restricted. An underlying document management system supports version control and a layer of metadata including comments on the reasoning behind edits. Because a Wiki is multiple-authored, attribution in a scientific sense is difficult. It can be the case that the meta-data available for any individual contributor does not allow any clear identification of their real identity or indeed credentials relevant to their contribution. This is a real issue for Wikipedia itself, and the extent to which the content contained there can be trusted. Many variations in the concept have evolved to address these various issues, including a commercial product known as Google Wave (*46*) (which was indeed explored as one mechanism for producing the present collection of articles you are reading at this moment). Regular Wiki pages have structured text, intended for humans to read and understand, and un-typed hyperlinks to other related pages. Semantic wikis use Semantic Web methods to address the search and information retrieval problems of Web 2.0 Wikis and its uncontrolled social tagging concept. Semantics may be either embedded within or separate from the Wiki markup. For example, a Semantic Wiki in medicinal chemistry could cover molecular targets within a particular disease area, such as oncology, and the compounds acting upon them. The page for one of these compounds would contain text information and semantic information, such as anti-carcinogenic properties, that a software agent would be able to disseminate. The Wiki would then be able to automatically generate a list of related compounds by listing all pages that are tagged with similar characteristics. Taking this simple notion to a more complex level, a Semantic Wiki could potentially support ontology reasoning and generate a complete ontology. Conversely, a Semantic Wiki can inherit a pre-existing ontology.

Semantic Wikis were first proposed in the early 2000s, and implementations emerged in the mid-2000s including the popular Semantic MediaWiki (*47*) (2005), Freebase (*48*) (2005) and OntoWiki (*49*) (2006). Most can export metadata as RDF. The application to chemistry has also been reviewed (*50*) and applied to an illustration of how an error in the molecular structure of mauveine might be automatically detected from information provided and structured within such a wiki (*51*).

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5.1.3. Podcasts

A podcast—the term being a merging of "iPod" and "broadcast"—is an audio or video recording which is uploaded to a "podcast feed" along with an RSS file containing metadata about the content and the author. Podcasts are created from Open Source or commercially available software. Participating Web pages would normally point to the feed location. Users subscribe to the podcast and are notified on their mobile devices (or docking station) whenever new content is available. In addition to iTunes, podcast search engines include Podscope and Odeo.

Podcast software normally support the two established versions of the RSS standard: RSS 2.0 (where RSS stands for "Really Simple Syndication") is an XML vocabulary where core metadata elements are defined within an XML schema. RSS 1.0 (where RSS stands for "RDF Site Summary") is based on RDF and can be processed by any RDF processor. The Dublin Core namespace is normally included. Additional XML namespaces are allowed by both versions but consideration needs to be made about how they would by handled by downstream applications. For example, if for scientific podcasts InChIs were included in the RSS, RSS 1.0 would be more appropriate as the podcasts could then be located on the Semantic Web.

A number of podcasts services for the chemistry community are provided by publishers. These include Nature's Chempod (*52*) and the RSC's Chemistry World Podcast (*53*). They are also used to some extent by individuals to disseminate lectures and accompanying notes. One of the present authors for example provides access to all their teaching, and a selection of their research lectures in this manner (*54*). In a related article (*55*), the merits of podcasts for chemistry lectures (along with the deficiencies of PDF) have been discussed. This article also discusses the value of incorporating CML into podcast RSS 2.0 metadata. RSS

A Semantic Web RDF vocabulary for podcasts, called Podcast Pinpointer has been published (*56*). This vocabulary uses as its basis RSS 1.0 along with Dublin Core and FOAF. Another RDF vocabulary which uses a modified version of Podcast has also been published (*57*). The synergy between these approaches and those of SemanticEye merit further investigation.

5.1.4. Social Networks

Social networks consist of a community of individuals with a common interest or purpose. The most popular social networking sites, including MySpace and Facebook, have millions of users. Normally a user would log on to a social network site and interact with its user interface to access a variety of services including email, instant messaging, picture and file sharing, blogging, and voice over IP. An alternative entry point supported by some social networks such as Twitter is text messages from mobile phones. A principal feature of social networks is the ability to rapidly create user groups against any topic of interest such as a geographic location or a scientific domain.

There are literally hundreds of social networks on the Internet and joining one normally requires registration and the creation of a public profile. Other more specialised social networks are open only to members of a particular group such as a place of work or a profession. A number of social networks, such as BiomedExperts (*58*), target a scientific membership. Profiles generally are site specific and need to be recreated for each site. At a given social network site, users would normally connect by searching the sites' metadata for names or other common features. Connections can be established by contacting "friends" directly or by joining groups. Most sites carry out local metadata interrogation in order to introduce users with common features to each other.

Because a FOAF is essentially social network metadata, the "inter-twingling" of FOAF and established social networks has been widely discussed and software tools exist which convert FOAF to and from formats understood by established social networks such as Facebook. Plaxo has been providing direct FOAF support for some time (*59*).

5.1.5. Mashups

A mashup combines data or functionality from two or more Web resources into a single service or presentation and normally targets the general public or the enterprise. Creating a mashup is usually straightforward involving open APIs and data sources used in manners that were not originally intended. Google Maps is an example of a resource with an open API that is frequently employed within mashups pertaining to locating specific entities. For example, a virtual venue for an electronic conference could be established as a mash up of a social network and a podcast feed. The notion that exposing content as RDF automates the mashup process has been investigated (*60*).

5.2. Project Prospect and ChemSpider

Project Prospect (*61*) is an RSC project to (semantically) enhance online journal articles. All of the RSC journals are in scope. Its goal is to make the science within RSC journal articles machine-readable through semantic enrichment by the annotation of key data and concepts within articles, such as compounds, and linking them to Web resources such as database objects. This will transform the free text within an article by adding new ways of identifying, retrieving and presenting the information within RSC publications.

One of the principal constituents of Project Prospect is the Experimental Data Checker (*62*) (OSCAR), a collaborative effort between Cambridge University and the Royal Society of Chemistry (RSC). Oscar follows a guiding principle that experimental molecular data is published in a consistent and predictable manner and this style does not vary much between journals and publishers. Regular expression parsing is performed on the manuscript, patterns and phrases in free text are identified, and some checks are then run to test the data for consistency. It can find molecular names and associate them to structures. The reported success rate of 92% is impressive.

As to who would ultimately sanction the tagging, a trained manuscript editor is obviously better qualified than the manuscript's author. If the manuscript has

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been submitted to a publisher, the manuscript editor would validate and ensure that the metadata is handled consistently in all the manuscripts. ChemSpider (*63*) is a free access chemical database which was released in March 2008 and acquired by the RSC in May, 2009. It provides access to millions of chemical structures and integrates to a variety of online services including the Wikipedia chemical structure collection. With over 21.5 million unique chemical entities, ChemSpider provides a foundation for a chemical document markup system. Chemical names are automatically identified within documents and Web pages and converted to chemical structures as InChI strings either algorithmically or by database retrieval. Although ChemSpider provides a Web interface to an extremely comprehensive collection of chemical resources, setting up a query within this Web interface to locate collaborators based on a molecule of interest is not straightforward. Semantic Web tools like SemanticEye can help, but molecular structures in ChemSpider would need to be represented as RDF via their InChI identifier. ChemSpider is currently moving in this direction; it is being integrated to rdf.openmolecules.net (*64*), a resource which provides autogenerated RDF for any InChI.

5.3. Reference Management Software

Reference management software enables scholars to record and track bibliographic citations. Once a citation has been recorded, it can be utilised in generating bibliographies for scholarly articles, books, etc. These packages normally consist of a database in which full bibliographic references can be entered. A selected list of articles can be formatted in the different formats required by publishers. Most packages provide a Microsoft Word plug-in to enable a reference list in the appropriate format to be produced automatically as an article is written. Other features include lookups of popular online libraries such as Google Scholar and PubMed. Bibliographic databases contain all article citations published in a particular discipline or group of disciplines, a prime example being the ISI Web of Knowledge (*65*). Reference management software suites are **not** bibliographic databases but they do all have the ability to import publication lists from the same.

Several of the more popular Reference Management packages are particularly noteworthy. Mendeley, which emerged in 2008, is one commercial attempt at providing reference management within a Web 2.0 social research environment. It essentially adapts the model of the popular social music service Last.fm where users share their listening habits and access the listening patterns of millions of other users to discover new artists or songs. Mendeley users are able to share and discover research patterns by publishing bibliographic lists. As with all Web 2.0 social networks, the Mendeley user base is built up through user invitations.

Users drag and drop research articles into a client and the articles are automatically uploaded to mendeley.com. Data and information mining algorithms then attempt to extract citation metadata from external resources, namely CrossRef, ArXiv, PubMed and Google Scholar, and from XMP metadata in the articles themselves if they exist. The articles may not yet have been published, in which case metadata may have to be added manually. The

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

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algorithms (which are not openly published) establish a scientist's expertise in a field by metadata interrogation as well by the number of times that articles are recommended. This concept of opening up a digital library with semantic metadata has also been rather picturesquely referred to as "defrosting" (*66*).

Zotero (*29*) is another well established reference management package available as Open Source. It provides many of the metadata management features of Mendeley. It also supports XMP extraction. However, Zotero differs in concept as it runs on the client as a Firefox plug in, and not a Web 2.0 application.

CiteULike (*67*), developed at the University of Manchester in 2004, was one of the earliest Web-based social bookmarking tools geared towards scientists. It is similar in concept to del.icio.us where users tag a document URI with metadata and share the tags online. The software is proprietary but the metadata it collects is openly available. Additional features include normalising tags for those articles that have been added by multiple users and determining the number of readers of a given article. Articles are normally accessed many more times than they are actually cited. CiteULike also incorporates metadata from EndNote and BibTeX.

6. Conclusions

In this article we reviewed how a strategic approach to metadata management for scientific electronic journal articles might provide mechanisms for new opportunities for collaborative interactions. The key requirement here is that scientific entities must be included in metadata and be readily searchable using established search standards. SemanticEye is an early exemplar of this notion with a focus on chemical electronic publishing and how the inclusion of molecular structures, uniquely defined as InChIs, within a Semantic Web metadata model can open up new vistas. By querying the SemanticEye ontology for InChIs using the SPARQL standard, communities of chemists based around common structures of interest can be automatically established. For example, representing such communities as FOAFs creates the possibility for reusing the communities within Web 2.0 social networking sites which understand FOAF thereby making these sites a viable alternative to electronic conferences for locating potential scientific collaborators. If a blog contained InChI representations of the molecules and/or the blogger's FOAF, the blog would link in to such communities. The same holds true for the scientific podcasts that includes FOAF elements and InChIs within RSS 1.0 metadata. In time, not only journals, but many other outlets for promulgating new ideas in science will acquire some degree of semantic content. The key point is that by formalising this semantic content, it will not be just humans that can participate in the process but also carefully constructed software agents that could act as proxies for the over-burdened human. This is indeed part of what Kurzweil (*18*) had in mind. In terms of teaching, one might imagine how a student of say chemistry might approach a body of lecture notes, blogs, journal articles and indeed iPad-optimized books (*68*) in which meaningful connections between the often diverse concepts are readily located. We hark back to the connections that it has taken one human a lifetime of teaching a course on pericyclic reactions to identify, as described in the first section above. But what of all the obvious connections that have been missed, and still need to be made? Perhaps the twenty year old world-wide information system that the Internet has become will eventually enable this too.

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Chapter 4

Web-Based Molecular Visualization for Chemistry Education in the 21st Century

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The Jmol molecular visualization project has anchored a revolution in the way we transmit and interact with chemical structure information on the Web. This chapter provides a brief history of that revolution and illustrates numerous ways Jmol has been integrated into Web sites that focus on chemical education. Subject areas covered include general chemistry, organic chemistry, crystallography, and inorganic chemistry.

Introduction

Chemistry has always been a visual science. From its early years in the late 19th century, the importance of the tetrahedron and the aromatic ring were recognized in organic chemistry. Through the years, understanding of the importance of stereochemistry in relation to physical and biological properties of small molecules, the helical nature of DNA and the three-dimensionally folded nature of proteins has been key to advances in chemistry and biochemistry. Today we have "molecular biology" which, of course, is really an extension of chemistry to biological systems that uses simple chemical reactions to effect amazingly complex biomolecular synthesis. And with these advances has arisen the need to communicate to students the three-dimensional character of bonding and molecular structure.

Chemistry, of course, like all sciences, has always been about communicating. For a long time, educators' sole means of communicating 3-D molecular structure in the classroom was through the use of wood or plastic models, and while there is much to say still for having a physical model *in hand*, the digital revolution of the late 20th century ushered in a totally new way of doing the business of chemistry

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education—a *virtual* way. The focus of this chapter is how this digital revolution has made possible a completely new way of teaching about molecular structure and function that takes the idea of a static hand-held model and gives it "life" in the largely unexplored virtual world of the World Wide Web. There are many aspects of this virtual world we do not yet understand, but a few things are clear: It is compelling, it is interactive, and it is enabling,

There were three dramatically new features of the digital revolution that particularly impacted chemistry education. First, for the first time, there was a medium that transcended the two-dimensional world of textbooks for transmitting to a wide audience the three-dimensional characteristics of the molecular world. Whereas prior to this revolution we had a few examples of idealized models—sticks arranged in the form of an ideal tetrahedron, trigonal planar models with precise 120 degree angles—now the diversity of molecular structure could be related in exquisite detail.

The revolution in terms of chemistry took off full speed with the introduction of the Chime Netscape Plug-in in 1996. Up to this point there was no reliable method of communicating three-dimensional molecular structure to students other than hand-held models and pretty two-dimensional figures. The Chime plug-in gave us for the first time a means of using virtual models to communicate molecular structure to a wide audience. And while one could argue as to its ultimate reliability—Chime required specific browsers with their own idiosyncratic features and never was developed for the Macintosh operating system—there is no question that Chime gave educators a feel for what was to be the future of molecular visualization. Despite all of its limitations, Chime was used for a wide variety of tutorials and Web-based educational projects for many years, and many sites still employ it, though, these days, probably without much of a following.

Second, for the first time, individual educators who had previously only dreamed of producing educational materials for the masses, or who had only marketed their masterpieces to their local clientele, were now empowered to produce materials that could be widely and *instantly* available to audiences far outside their traditional circle of colleagues and students.

Perhaps most significantly in relation to this revolution, with the advent first of list servers and more recently with blogs and wikis, educators and students have become connected in ways that only twenty years ago would have been absolutely impossible. Most importantly for the discussion at hand, there arose a widely dispersed core of educators and largely self-trained Web designers who mastered the nuances of the Web and started building the next generation of educational materials based on the principles of open access, open source, and community development.

Over the past few years the advances in molecular visualization have been nothing less than outstanding. While we are still learning new ways of capitalizing on this highly distributed technology, at this point in time it is interesting to take a look at where we are and what capabilities we now have at our fingertips.

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The Jmol Molecular Visualization Project

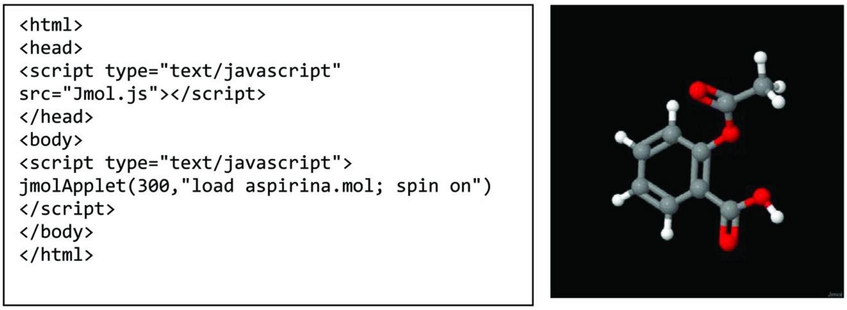
The Jmol Molecular Visualization Project, one of the early open-source projects of the 1990s really came of age in 2002 when it became the de facto replacement for Chime, which had lost its commercial development support, was not released to the public domain, and could not keep pace with the rapidly developing browser market. In contrast to Chime, Jmol presented the opportunity for a rapidly developing program within a dedicated community of users and developers,

Jmol has in the past several years grown from its initial focus as a Web-based RasMol/Chime replacement into a powerful visualization and analysis tool that remains highly modular and customizable. Unlike the other programs of the previous century, Jmol is essentially a massive easily accessible toolbox that can be used at the lowest level by dedicated professional Java programmers wanting to integrate molecular visualization into larger projects, at a more common level by scientists and educators wishing to communicate information via the Web, and, finally, by students with little or no Web design experience in the context of class projects, tutorials, and laboratory exercises.

Integrating 3-D Models into a Web Page

Addition of 3-D molecular models into a Web page is simplicity itself. The HTML code in Figure 1, for example, displays a model of caffeine and starts it spinning slowly, provided the standard set of Jmol JAR (Java archive) files, Jmol.js, and aspirina.mol are in the directory containing the Web page:

A wide variety of file formats are readable by Jmol. The full list is available at the Jmol interactive documentation site (*1*). Table 1 summarizes only a few of the most common of the more than 40 file formats available.



```
<html>
<head>
<script type="text/javascript"
src="Jmol.js"></script>
</head>
<body>
<script type="text/javascript">
jmolApplet(300,"load aspirina.mol; spin on")
</script>
</body>
</html>
```

Figure 1. A very simple Web page showing a molecule in 3-D using the Jmol applet. (see color insert)

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Table 1. Selected structure file formats readable by Jmol

cif	Crystallographic Information Files—the standard file format for crystallography (*2*).
jme	Java Molecular Editor 2-D files; Jmol will use an algorithm to create a 3-D object from the 2-D data (*3*).
mo	WebMO format files, describing atom positions, bonding, and molecular orbitals, which can also be calculated and displayed via a Web-based interface that utilizes an embedded Jmol module for its molecular rendering (*4*).
mol/sdf	Symyx molfile/SDfile format includes atoms, formal charges, and multiple bonding (*5*).
pdf	Protein Data Bank files. This relatively simple file format can also be used for small molecules and includes a generic data field that can be used for coloring atoms or surfaces (*6*).
smol	structure files created by Spartan. These files may contain additional data, including fractional charges, molecular orbitals, and calculated vibrational modes (*7*).
xyz	atom positions only; single bonding supplied by Jmol. Multiple models may include vibrational modes or coordinate animation information (*8*).

```
<script type="text/javascript">
jmolApplet(400,"load aspirina.mol;")
jmolBr()
background: jmolLink("background
white","white")
jmolHtml(" ")
jmolLink("background black","black")
jmolRadio("spacefill","spacefill", false, " ")
jmolRadio("wireframe 0.15;spacefill
23%","ball&stick", true, " ")
</script>
```

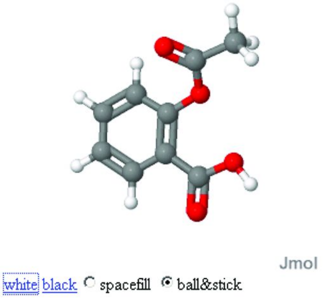

Figure 2. Providing a few viewing options. (Only the body of the HTML is shown.) (see color insert)

Adding Interactivity

While there are occasions when one simply wants a model of a molecule that can be manipulated or spun, the real power of Jmol lies in what you can do around it. The general functionality includes buttons, checkboxes, option (or "radio") buttons, hypertext links, drop-down menus, and an optional command input box. These features are very simple to configure and allow the Web page visitor to quickly view the model in a variety of pre-set ways (Figure 2). Full details are available at the Jmol Wiki (*9*).

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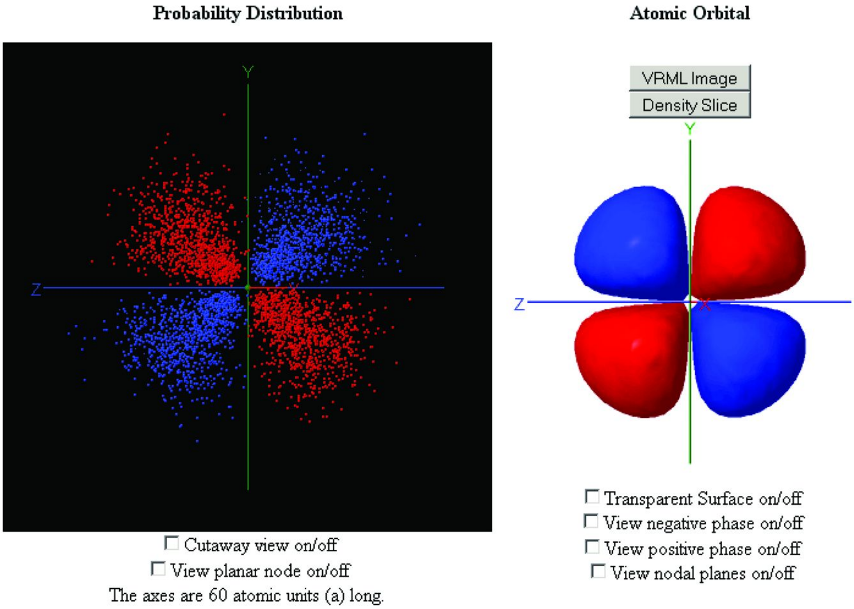
Full Interactivity

For more sophisticated interactivity one needs to use a bit of JavaScript. Jmol's design includes a wide collection of "callback" functions that allows the Web page to be notified when events such as file loading, mouse movement, and atom picking take place or when messages or errors are generated by the scripts running in the applet. The full list of callback capabilities are given in the Jmol documentation. In addition, designed into Jmol is a rich mathematical scripting language that allows querying of the model—distances, bond angles, charges, selections of atoms, volumes contained by surfaces, relative orientations of molecules, descriptions of space group and point group symmetry elements—essentially every aspect of the model. Ultimately, Jmol can be used to create highly interactive applications that incorporate three-dimensional structure in ways that are essentially only limited by the creativity of a JavaScript-savvy Web page designer.

In the next section we take a look at a few of the hundreds of education-oriented Web applications that have been designed specifically around Jmol to take advantage of some of its more sophisticated capabilities. We focus here on the areas of general chemistry, organic chemistry, and inorganic chemistry. In every case the functionality of Jmol that is highlighted was suggested by one or more users in the Jmol open-source community and implemented within days or weeks of the request.


Probability Distribution
Atomic Orbital
VRML Image
Density Slice
Y
Z
X
Y
Z
X
☐ Cutaway view on/off
☐ View planar node on/off
☐ Transparent Surface on/off
☐ View negative phase on/off
☐ View positive phase on/off
☐ View nodal planes on/off

The axes are 60 atomic units (a) long.

Figure 3. Interactive 3-D representations of atomic orbitals using a probabilistic representation (left) and the standard "isosurface" (right). In color, the lobes are alternately red and blue. (see color insert)

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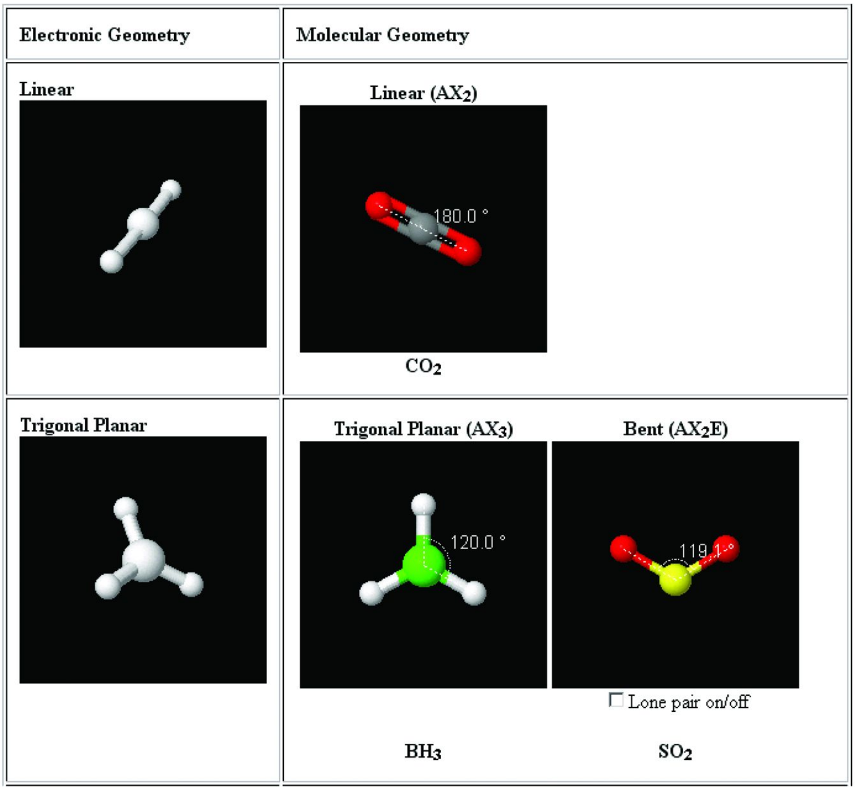

Electronic Geometry	Molecular Geometry	
Linear	Linear (AX_2) CO_2	
Trigonal Planar	Trigonal Planar (AX_3) BH_3	Bent (AX_2E) ☐ Lone pair on/off SO_2

Figure 4. A table of Jmol applets organizing molecular geometries in terms of their corresponding electron pair geometries. Three additional rows illustrate tetrahedral, trigonal bipyramidal, and octahedral geometries. (see color insert)

Visualizations for General and Inorganic Chemistry

The primary interest in Web-based molecular visualization in general and inorganic chemistry has been in the depiction of atomic and molecular orbitals, and the description of molecular geometry in terms of VSEPR theory. A particularly interesting depiction of atomic orbitals can be found at the *Chemistry the Central Science* site (*10*) from Ohio State University (Figure 3). This site uses many of the simple interactivity features discussed above to excellent effect. The probabilistic representation on the left is accomplished using a simple pre-calculated XYZ file that is really about 30-times scale, and assigning N atoms to one orbital phase and C atoms to the other, then coloring those as desired.

Also at this site is a highly effective discussion of molecular shapes in relation to VSEPR theory (*11*) (Figure 4). Notice in this case the use of Jmol "measures" to emphasize the bond angles, and the use of a table of applets to organize molecular shapes along the lines of their corresponding electron pair geometries. For SO_2, an option to show the lone pair illustrates the relationship of the shapes in any given row. Visualization of other molecular properties such as molecular electrostatic potential maps, molecular orbitals, vibrational normal modes, and symmetry elements is possible at the Chemical Education Digital Library *Models 360* site (*12*) (Figure 5). Also associated with the ChemEd DL is *Periodic Table Live!*, which uses Jmol to present crystal structures of the elements (Figure 6).

Visualizations for Organic Chemistry

Clearly a rich area for visualization is the study of organic chemistry. Discussions of stereochemistry, conformational changes, electron delocalization, and reaction pathways just to name a few all require some understanding of the three-dimensional character of the molecular world. Historically it has been a part of the rite of passage through organic chemistry to get a model set and work with it to bring the static images of the textbook into some sort of three-dimensional reality. One relatively recent solution to this educational challenge is to move to an interactive online textbook where the illusion of 3-D can be accomplished far better than on paper. A prime example is the *Virtual Textbook of Organic Chemistry* (*13*), which was developed during the Chime era and beautifully integrates that technology into the discussion. Recently this site has been converted to using Jmol—a relatively simple operation only requiring the insertion of two lines of HTML code into the page (*14*). This immense project has been a tremendous contribution to the undergraduate study of organic chemistry. Another comprehensive resource is *Mol4D* (*15*), a topic-oriented set of on-line tutorials focusing on organic chemistry. One of the interesting aspects of this work is that all of the models and animations are results of calculations. Figure 7 shows one such animation that proves that the boat conformation is not a required step along the path between two corresponding chair conformations of cyclohexane—a point not typically made in standard textbooks.

One of the areas most amenable to Web-based illustration is that of organic reaction mechanisms. A fore-runner in this area is *ChemTube3-D* (*16*), out of the University of Liverpool (Figure 8). The philosophy here is that the student user can choose to look at the structure of the reactants, the products, or the reaction that takes one to the other. The clever interface uses an HTML image map to drive a Jmol animation between its end points.

It is even possible that we are now in a position to say that the need for a plastic molecular model kit in organic chemistry is nearly a thing of the past. With the recent introduction of the Web-based *Jmol Molecular Model Kit* (*17*) (Figure 9), students for the first time can construct their own 3-D molecules and investigate them *by drawing in 2-D*. The 2-D coordinates and stereochemical information are passed from the Java Molecular Editor (*3*) to Jmol via JavaScript. This almost magical experience utilizes Jmol's powerful yet very fast Universal Force Field (*18*) implementation.

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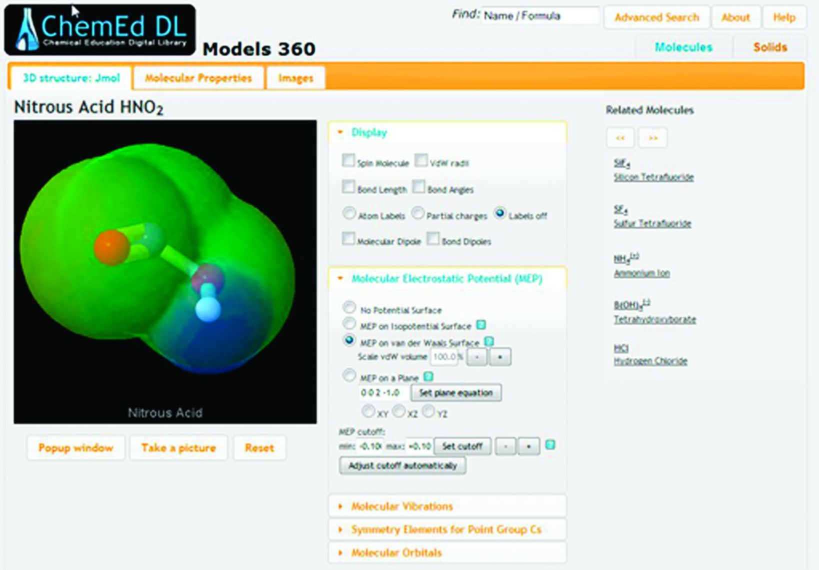
ChemEd DL
Chemical Education Digital Library
Models 360
Find: Name / Formula
Advanced Search
About
Help
Molecules
Solids
3D structure: Jmol
Molecular Properties
Images
Nitrous Acid HNO_2
Nitrous Acid
Popup window
Take a picture
Reset
Display
Spin Molecule
VdW radii
Bond Length
Bond Angles
Atom Labels
Partial charges
Labels off
Molecular Dipole
Bond Dipoles
Molecular Electrostatic Potential (MEP)
No Potential Surface
MEP on Isopotential Surface
MEP on van der Waals Surface
Scale vdW volume 100.0%
MEP on a Plane
0 0 2 -1.0
Set plane equation
XY XZ YZ
MEP cutoff:
min: -0.10 max: +0.10
Set cutoff
Adjust cutoff automatically
Molecular Vibrations
Symmetry Elements for Point Group Cs
Molecular Orbitals
Related Molecules
SiF_4 Silicon Tetrafluoride
SF_4 Sulfur Tetrafluoride
$NH_4^{(+)}$ Ammonium Ion
$B(OH)_4^{(-)}$ Tetrahydroxyborate
HCl Hydrogen Chloride

Figure 5. The Chemical Education Digital Library Models 360 site. (see color insert)

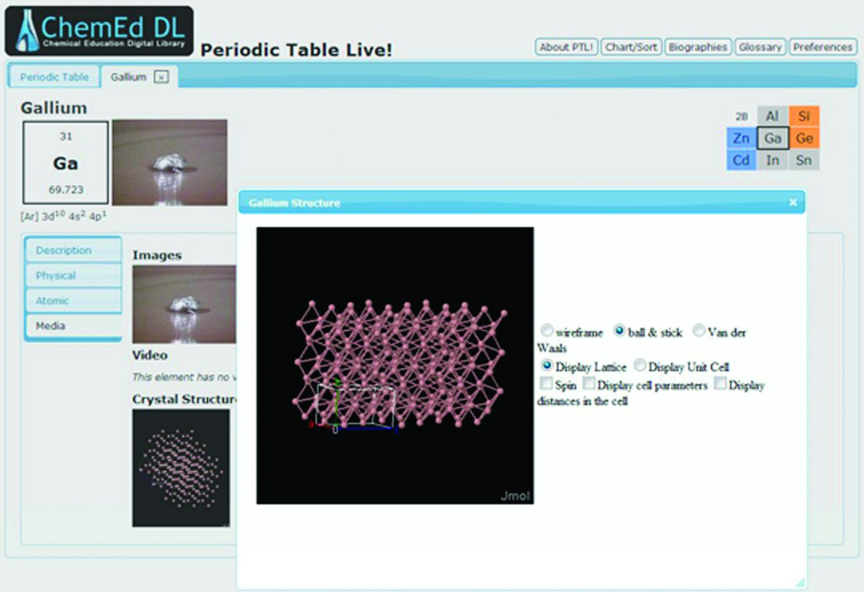
ChemEd DL
Chemical Education Digital Library
Periodic Table Live!
About PTL!
Chart/Sort
Biographies
Glossary
Preferences
Periodic Table
Gallium
Gallium
31
Ga
69.723
[Ar] $3d^{10}$ $4s^2$ $4p^1$
Description
Physical
Atomic
Media
Images
Video
This element has no
Crystal Structur
28
Al
Si
Zn
Ga
Ge
Cd
In
Sn
Gallium Structure
Jmol
wireframe
ball & stick
Van der Waals
Display Lattice
Display Unit Cell
Spin
Display cell parameters
Display distances in the cell

Figure 6. Chemical Education Digital Library's Periodic Table Live! (see color insert)

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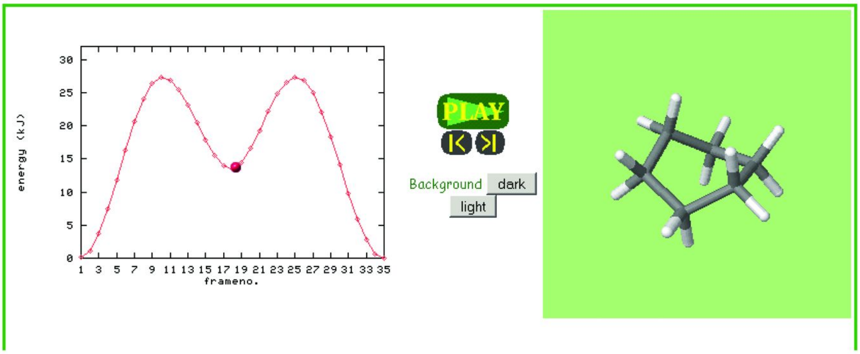
30
25
20
15
10
5
0
energy (kJ)
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35
frameno.
PLAY
|< >|
Background dark
light

Figure 7. A Jmol animation that uses mouse-click callbacks to synchronize the graph on the left with its corresponding conformation on the right. (This snapshot is of the twist boat.) (see color insert)

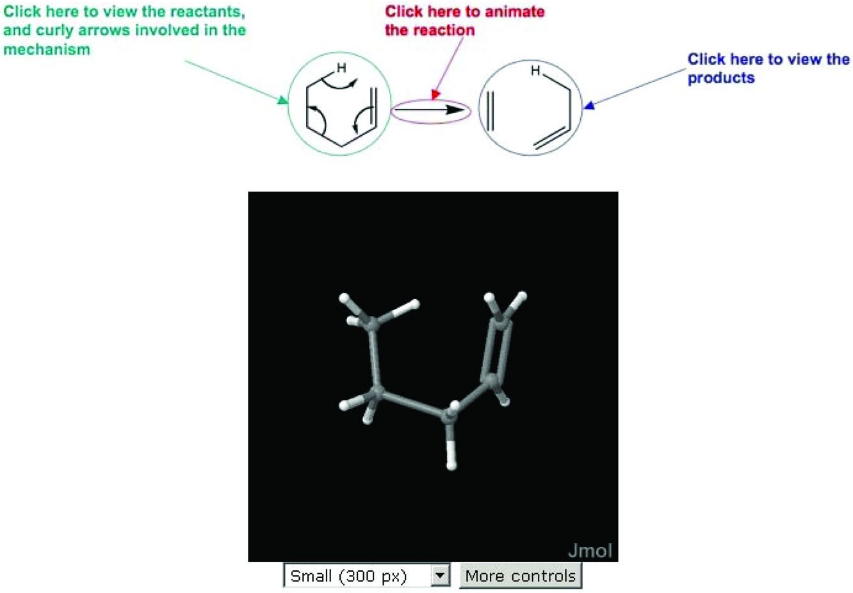
Click here to view the reactants, and curly arrows involved in the mechanism
Click here to animate the reaction
Click here to view the products
H
H
Jmol
Small (300 px)
More controls

Figure 8. Using an image map to direct Jmol through an animation. (see color insert)

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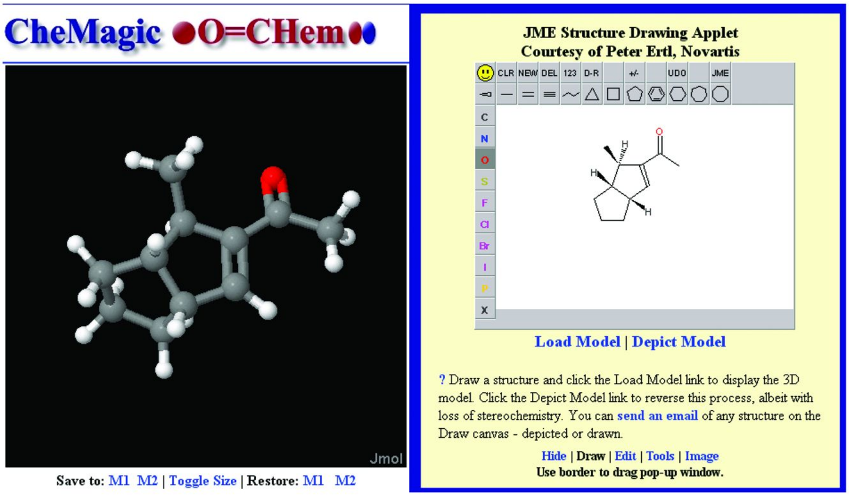
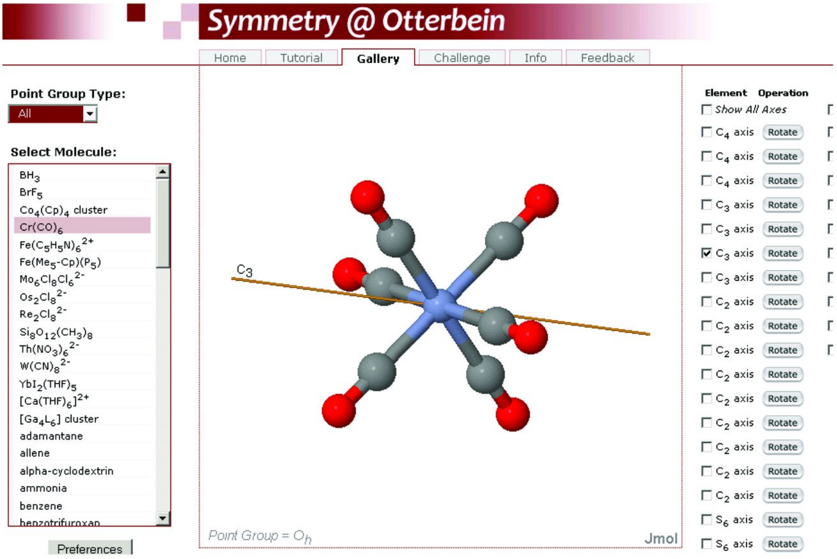

CheMagic ●O=CHem●●
Jmol
Save to: M1 M2 | Toggle Size | Restore: M1 M2
JME Structure Drawing Applet
Courtesy of Peter Ertl, Novartis
CLR NEW DEL 123 D-R +/- UDO JME
C
N
O
S
F
Cl
Br
I
P
X
O
H
H
H
Load Model | Depict Model
Hide | Draw | Edit | Tools | Image
Use border to drag pop-up window.

? Draw a structure and click the Load Model link to display the 3D model. Click the Depict Model link to reverse this process, albeit with loss of stereochemistry. You can send an email of any structure on the Draw canvas - depicted or drawn.

Figure 9. 2-D to 3-D conversion using the Java Molecular Editor in association with Jmol. (see color insert)


Symmetry @ Otterbein
Home
Tutorial
Gallery
Challenge
Info
Feedback
Point Group Type:
All
Select Molecule:
BH_3
BrF_5
$Co_4(Cp)_4$ cluster
$Cr(CO)_6$
$Fe(C_5H_5N)_6^{2+}$
$Fe(Me_5\text{-}Cp)(P_5)$
$Mo_6Cl_8Cl_6^{2-}$
$Os_2Cl_8^{2-}$
$Re_2Cl_8^{2-}$
$Si_8O_{12}(CH_3)_8$
$Th(NO_3)_6^{2-}$
$W(CN)_8^{2-}$
$YbI_2(THF)_5$
$[Ca(THF)_6]^{2+}$
$[Ga_4L_6]$ cluster
adamantane
allene
alpha-cyclodextrin
ammonia
benzene
benzotrifuroxan
Preferences
C_3
Point Group = O_h
Jmol
Element Operation
☐ Show All Axes
☐ C_4 axis Rotate
☐ C_4 axis Rotate
☐ C_4 axis Rotate
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☐ C_2 axis Rotate
☐ C_2 axis Rotate
☐ C_2 axis Rotate
☐ S_6 axis Rotate
☐ S_6 axis Rotate

Figure 10. The Symmetry Gallery. Every point group relevant to chemistry is represented, and all symmetry elements can be depicted and activated. (see color insert)

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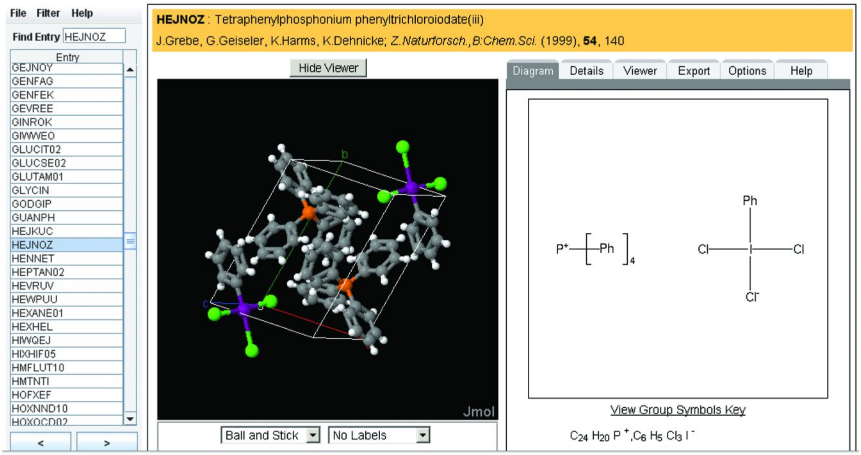

HEJNOZ : Tetraphenylphosphonium phenyltrichloroiodate(iii)
J.Grebe, G.Geiseler, K.Harms, K.Dehnicke; *Z.Naturforsch.,B:Chem.Sci.* (1999), **54**, 140

Find Entry HEJNOZ

Ball and Stick
No Labels

File Filter Help
Entry
GEJNOY
GENFAG
GENFEK
GEVREE
GINROK
GIWWEO
GLUCIT02
GLUCSE02
GLUTAM01
GLYCIN
GODGIP
GUANPH
HEJKUC
HEJNOZ
HENNET
HEPTAN02
HEVRUV
HEWPUU
HEXANE01
HEXHEL
HIWQEJ
HIXHIF05
HMFLUT10
HMTNTI
HOFXEF
HOXNND10
HOXOCD02
<
>
Hide Viewer
b
c
Jmol
Diagram
Details
Viewer
Export
Options
Help
P⁺
Ph
4
Ph
Cl
I
Cl
Cl⁻
View Group Symbols Key
C24 H20 P⁺,C6 H5 Cl3 I⁻

Figure 11. The Cambridge Crystal Database uses both 3-D and 2-D molecular visualization. (see color insert)

Visualizations for Crystallography and Inorganic Chemistry

Some of the most interesting work in Web-based visualization has been in the area of inorganic chemistry. Crystallography, symmetry, surfaces, inorganic complexes—all involve discussions that require mastery of the not-so-simple three-dimensional character of metal-centered bonding. These areas are representative of just how powerful open source is when there is an active user group. Two contributions by this author, *Cool Molecules* (*19*) and *The Jmol Crystal Symmetry Explorer* (*20*) were both developed synergistically with Jmol. Prior to *Cool Molecules*, Jmol could not load model data directly calculated on a Web site rather than stored in server-based files; prior to the development of the *Jmol Crystal Symmetry Explorer*, Jmol could not depict crystallographic symmetry operations that relate selected atoms or molecules. These developments in visualization were driven by the dynamic nature of the open-source Jmol user community.

In terms of point group symmetry, the development of *Symmetry Resources at Otterbein College* (*21*) (Figure 10) has pushed Jmol's development more than any other. It is notable that the page loads a model file using Jmol, and then Jmol *itself* determines the space group and reports all symmetry operations.

As a final example, the Cambridge Crystallographic Database has recently introduced an interactive teaching tool, a component of WebCSD (*22*) that focuses on crystal structures and how they can be used to investigate trends in bonding (Figure 11). While the site itself is rather complex, the addition of the Jmol applet for purposes of visualization was straightforward.

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Summary

Needless to say, this is just a small sampling of what is available in terms of Web-based molecular visualization. 3-D interactive molecular visualizations can contribute also to blogs (*23*) and wikis (*24*). There are hundreds of additional pages that actively present molecular systems in a way that is simple to introduce and seamless in its integration with the other "value-added" features of the Web page. In addition, none of the hundreds of Web sites in the area of biochemistry and structural biology have been presented here. Additional uses involve Web-based molecular visualizations at the "front-end" of databases, which of course make major contributions to chemical and biochemical education as well as industry and research. Examples include ChemSpider (*25*), the ChemExper Chemical Dictionary (*26*), the Inorganic Crystal Structure Database (*27*), the American Mineralogist Crystal Structure Database (*28*), the Protein Data Bank (*29*), and the Jena Library of Biological Macromolecules (*30*).

It is a testament to the open-source movement (*31*) that much of the development in the area of Web-based molecular visualization has come from ideas generated in the wider open-source community in a context of open and productive dialogue between developers, researchers, and educators. This is truly a new paradigm for 21st century science.

Acknowledgments

It is not possible to thank all of the people who have made contributions to the Jmol project. Dan Gezelter was the original developer of Jmol to whom we are all very much indebted. Several other programmers contributed over the years, most notably Egon Willighagen, Nico Vervelle, René Kanters, and especially Michael (Miguel) Howard. Innumerable Jmol users have contributed ideas, designs, and solutions to problems over the years. Special thanks go to Tim Driscoll, Jonathan Gutow, Sidney Hall, Angel Herráez, Alan Hewat, Dean Johnston, Brian Martz, Brian McMahon, Frieda Reichsman, Peter Murray-Rust, among many, many others.

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Chapter 5

Wikipedia as a Resource for Chemistry

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Wikipedia has become a valuable reference source—too important to ignore, yet often poorly understood in the academic community. This chapter describes how chemical educators, chemists and students can use this vast resource, wisely and with a critical eye, when researching for routine work, papers or term projects. It explains how the chemistry content on Wikipedia is written, organized and checked, and how the articles are laid out. The text describes several useful strategies when using Wikipedia to find specific types of information. It also explains how to design writing assignments based on students' contributions to Wikipedia.

What Wikipedia Is, and Why It Matters

Wikipedia has transformed the world of information, bringing (in effect) a room full (*1*) of encyclopedia volumes to our desktops. It provides information on everything from Ethiopian towns to episodes of "The Simpsons"—often with clickable references. Not surprisingly, it has become the most popular information resource on the Internet (*2*), with about 13% of all Internet users using Wikipedia in a typical day (*3*). Yet it remains poorly understood.

Wikipedia defines itself as "a free, Web-based, collaborative, multilingual encyclopedia project supported by the non-profit Wikimedia Foundation." (*4*) *Free* in this context means that its content can be re-used and modified with few legal restrictions. The mission of the Wikimedia Foundation (WMF) also states its commitment to "make and keep useful information from its projects available on the Internet free of charge, in perpetuity." (*5*) Its vision is a lofty one: "Imagine a world in which every single human being can freely share in the sum of all knowledge." (*6*) These aims have fostered a culture where thousands of individuals

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

are willing to donate their time and knowledge, free of charge, to build Wikipedia into the resource it is today.

Wikipedia differs radically from traditional information resources, since it "favors consensus over credentials in its editorial process" (*4*). In place of a single "expert" to write articles, Wikipedia uses a system of open editing by those members of the general public who choose to participate. These contributors freely and continually change the work previously uploaded, with content approaching a hypothetical "ideal state" asymptotically. Disputes are resolved through open discussions guided by five basic principles or "pillars," such as "neutral point of view," and also a detailed Manual of Style (*7*). For articles that have a large number of contributors, at least, Wikipedia epitomizes the idea of "crowdsourcing" and "wisdom of crowds" (*8*) to develop a level of balance and expertise. This outcome can be seen in a 2009 survey of expert toxicologists, which found that Wikipedia was considered one of the most balanced sources of toxicology information, and much more reliable than the traditional media (*9*). Being a dynamic community with information stored electronically, it can also correct errors quickly. The community can continually develop, and even change how the quality of information is defined (*10*).

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This approach is not, however, without its detractors. Some criticisms stem from oversimplification or misunderstanding, as captured in TV comedy *The Office*, where character Michael Scott states sarcastically: "Wikipedia is the best thing ever. Anyone in the world can write anything they want about any subject, so you know you are getting the best possible information" (*4*). This fallacy is based on the idea that the majority of editors are attempting to add misinformation, or write with only a puerile understanding of the topic. Although such editors are not uncommon, the reality is that most users find Wikipedia to be a useful resource. How is that possible? Priedhorsky *et al* found that rogue contributions are usually removed or corrected (*11*) very quickly, commenting that the fact that the Wikipedia system works is "amazing." Viegas *et al* found that "the community maintains a strong resilience to malicious editing" (*12*). Nevertheless, errors and vandalism can persist unnoticed, sometimes for a long time (*13*), particularly in cases where the misinformation may appear credible, or if it is on a page that is little read. Pages with political or commercial ramifications may be heavily edited by people with a strong bias. The Wikiscanner site (*14*) was created specifically to allow the public to check for edits by biased sources, and its results are quite revealing (*15*).

So can the information be trusted? Can a scientist or student rely on the information to be accurate? Obviously, Wikipedia's methods suffer from a "credibility gap". Although a 2005 study by Nature famously found little difference in reliability in scientific articles between Wikipedia and Encyclopedia Britannica (*16*), both sources were found to have many omissions and errors. The GMU toxicology survey (mentioned above) still only rated Wikipedia as 45% accurate. As Lankes has noted (*17*), the Web has caused a shift in how information is assessed by users; credibility is increasingly determined by *reliability* rather than traditional forms of authority. If Wikipedia works for me, why shouldn't I use it?

The lesson is clear; *all* information sources should be regarded with a critical eye. It may be that we have allowed ourselves to believe that the expert-based system for producing scientific information is objective and free of errors. We prefer to ignore cases of poor reviewing, cronyism and outright fraud that have always compromised traditional information sources. Wikipedia has its faults, but it is not alone in this, and we should apply the same standards to all of our resources.

But the most important lesson is more basic—Wikipedia is an incredibly valuable and significant resource, and we would be neglecting our students if we tried to pretend it wasn't there. Why should we tell students not to use Wikipedia, when we all use it ourselves? As Cathy Davidson states in her 2007 opinion piece in the *Chronicle of Higher Education*, "We can't ignore the influence of digital technologies." (*18*) Rather, we need to learn how to use Wikipedia carefully, then convey this to our students. This is best done by understanding how the Wikipedia community works, and how the information is organized; these topics make up the remainder of this chapter.

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What Wikipedia Is Not

Misunderstandings about the nature of Wikipedia are as common as the criticisms; these are addressed on the Wikipedia page, "Wikipedia:What Wikipedia is not." (*19*) These include:

- *Wikipedia is not a publisher of original thought.* It is also *not a textbook or scientific journal.* Many chemists seem to believe that they will be able to disseminate their research through a Wikipedia article. In practice, Wikipedia has quite a conservative policy on what is allowed as an article topic. For example, a new scientific idea must be both published and at least partially accepted within the scientific community before it will be considered as appropriate for Wikipedia. The threshold for inclusion in Wikipedia is **verifiability, not truth**—whether readers can check that material in Wikipedia has already been published by a reliable source, not whether editors think it is true (*20*).
- *Wikipedia is not an indiscriminate collection of information* and *Wikipedia is not a soapbox or means of promotion*. Any article must be seen as "notable"—a slippery concept, perhaps, but "vanity articles" or opinion pieces are swiftly deleted by the Wikipedia community.

In addition to the above, I have often encountered a misconception that Wikipedia is written almost entirely by children and amateurs. I would therefore like to add my own "not" statement:

- *Wikipedia chemistry articles are not written by kids who have little understanding of what they write about.* The Wikipedia grassroots community respects one thing above all else—the ability to write high quality content. If a person's edits indicate that the contributor has a good grasp of the topic, the contributions will remain and that person

> will quickly earn the respect of other chemistry editors. If the edits are poor, they will be altered or removed, and the person will typically leave or work on topics where their contributions are more valued.

The sort of person who spends time writing about a topic such as molybdenum hexacarbonyl is usually someone who understands it and cares about it. I have personally met several of the most prolific contributors to the chemistry content on Wikipedia. Some are professional Ph.D. chemists (or were until retirement)—college professors and industrial chemists. Some are undergraduate students—but typically these are the brightest and best of their peers, and in general their contributions are also of high quality. Most important, there is an active, friendly community of chemists which ensures that most content undergoes a certain amount of "peer review". (Of course, controversies arise, but the chemistry community has a history of resolving such things amicably, as can be seen from article and WikiProject discussion pages; this is not true, however, for all groups on Wikipedia.).

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How Wikipedia Chemistry Articles Are Written

Most new contributors begin with small changes to existing articles. Writing begins with the "Edit" tab at the top of every Wikipedia page—visible to all users on most articles (*21*). Text can simply be added or deleted as needed. The Wikimedia software running Wikipedia does not provide WYSIWYG editing, but nevertheless it is fairly easy to master, and most readers of this book would have little trouble in making basic edits. The toolbar assists the editor with all common operations, and even the complex task of adding a reference. A preview option allows checking before changes are saved—useful for making sure that your edit does not cause the article format to "break"! Every previous version of the article can be viewed via the History tab and (if necessary) restored, so any erroneous edits can be easily reverted.

Before a major change is made to a page, it is usual first to discuss the change on the article's discussion page (accessed via the discussion tab). In this way discussions take place in a separate place from the article content, and blunders can be avoided (such as a British editor trying to rename the *Sulfuric acid* article as *Sulphuric acid*). These discussion pages form a permanent record (including archives), and they can often provide insights into why the article is written the way it is (*12*).

If a completely new article is required, this can be done by typing the proposed article name into the search box and typing "Go"; if there is no article containing the name the user will be asked if they want to create an article with that name (shown in red). If articles exist containing the proposed name, these will be listed. This can be useful in cases where synonyms exist, but there is no "redirect" page—a page that simply redirects the user from one page name to another, such as from DMSO to dimethyl sulfoxide. Completely new articles of significance are often discussed at the relevant WikiProject (see below) to ensure that the topic is appropriate, and that the content is well-written and balanced.

These same projects maintain the "Manual of Style" for writing chemistry articles (*22*), which is used to guide editors in how to name substances, draw structures, etc.

How Wikipedia Chemistry Content Is Organized

The Wikimedia software provides a simple hierarchical system for organizing content, based on *categories* (*23*). Chemistry articles can be loosely defined as being articles that come into a subcategory of Category:Chemistry, though this definition takes in many non-chemistry articles too (*24*). Categories can be found at the bottom of almost any Wikipedia article, and clicking on the category takes the user to a page listing all articles in that category. This is most useful when the category has a clear scope, for example Category:Selenium compounds.

Graphical information, such as photographs, graphs and charts, is stored in separate files that are "transcluded" into the article from a separate location, often on the Wikimedia Commons (*25*). This allows the same image to be used in many articles in many different languages, with each page loading in the image at only the desired size, thereby saving bandwidth. One weakness of transclusion, however, is that if an image file is changed (possibly through vandalism) there is no record of that change on the page where the image is being used.

Chemistry content is loosely overseen by the Chemistry WikiProject (*26*) (for general topics on chemistry), the Chemicals WikiProject (*27*) (for articles on specific chemical compounds) or the Elements WikiProject (*28*) (chemical elements). Chemistry-related content is also often handled by the Pharmacology WikiProject (*29*) (mainly drugs), the Molecular and Cellular Biology WikiProject (*30*) (much biochemistry) the Geology WikiProject (*31*) (which oversees minerals) and the Physics WikiProject (*32*) (covering some chemical physics). Chemistry articles can be defined as those articles which carry a template tag from one of these WikiProjects on their discussion pages, although a few chemistry articles may be missing such tags. These templates also generate discussion page categories; these are used mainly for assessment, but they allow changes to be logged, and article metadata can be tracked and summarized (*33*). These projects mainly work on defining standards and reviewing/improving articles within their subject area, but occasionally they may also launch other initiatives, such as collaborations with external organizations.

Chemical substance articles tend to follow a fairly standard format (*34*). As with all Wikipedia articles, the page begins with a lead section or "lede," giving an overview of the topic. This is typically followed by sections covering physical and chemical properties, synthesis, reactions and applications. Most substance pages also contain a "Chembox" which summarizes the main data relating to the substance, such as structure, CAS Registry number, or melting point. The Chembox is organized into sections covering different aspects: identifiers (e.g., CAS#, InChI), properties (e.g., formula, melting point), structure (crystal structure), hazards (summary only, with a link to an external MSDS) related compounds, and supplementary data. This last section links to a separate page which gives more specialized information, for example spectral information,

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vapor pressure curves, etc., which are useful but which might clutter up the main article page. The Chembox has evolved into quite a sophisticated template, where (for example) molar masses are automatically calculated from the formula). Chemical elements have a similar "Elementbox" and drugs use a "Drugbox" to summarize pharmacological information.

Organic functional groups do not have a databox, but usually contain certain sections: lead, structure, nomenclature, reactions and synthesis. Likewise, organic reactions often follow a standard format (*35*). After an overview of the reaction, the mechanism is often given, and the scope and variations; where relevant, stereochemistry or regiochemistry may be discussed, and there is usually a list of useful reviews. Named reactions are often covered well, but unnamed transformations (such as aldehyde to carboxylic acid) frequently have no article.

Most other types of chemistry article are harder to classify, and are less uniform in format. This also makes the articles more difficult to write, especially where the subject is broad, so the coverage of such topics can be patchy. Articles on chemists and chemical businesses are often quite weak, especially (on the English Wikipedia) for those outside the English-speaking world.

Validation of Wikipedia Content

Now that Wikipedia has become one of the world's major resources for chemical information, it has become imperative that the quality of the information be improved. Thousands of chemists rely on Wikipedia every day, and many students trust it as they write their papers and study for their exams. More than that, one emergency responder has informed me that paramedics often use Wikipedia for drug information, since they find it to be up-to-date and quite reliable. This puts an immense burden of responsibility on a small group of volunteers—to maintain and improve the reliability of information in a vast (and growing) resource that is open for anyone to edit.

Fortunately, the Wikipedia model comes with built-in checks and balances. Vandalism is often corrected immediately by the "Vandalism Patrol", or by automated scripts called "bots"; no chemistry knowledge is needed for spotting most vandalism! When there is uncertainty about specific facts, discussion pages allow people to reach a consensus (*36*). A questionable statement can be quickly tagged with "citation needed" (*37*), and other similar tags indicate that the article requires cleanup.

The real challenge is to raise the standard of data on Wikipedia above the mediocre, something which requires a formal process of curation and validation (*38*). In effect, validation asks the question, "How can I be sure that this information is correct?" Late in 2007, Dr. Antony Williams of ChemSpider began working through a database of Wikipedia chemical substance articles (*39*), performing a rigorous check of every Wikipedia structure in the database against ChemSpider, PubChem, and other databases (*40*). He reported any errors, and chemists from the Wikipedia community then set to work to fix the problems (*41*). Although this curation cleared up many simple errors or omissions, it became clear that many online errors might be perpetuated -for example, if Wikipedia takes an erroneous structure from PubChem, and the same structure has been deposited at ChemSpider, as many of these databases reference each others' data. After an extensive series of online meetings (*42*) (held using Internet Relay Chat or IRC), a more formal validation effort of chembox and drugbox data was initiated, building on Williams' initial work (*43*).

The initial goal of the validation effort appeared modest—to ensure the veracity of the structure, IUPAC name, formula and CAS Registry Number. This goal was achievable with a core group of around four members of the Wikipedia chemistry community. These few data fields provide a foundation upon which future validation efforts can be built; clearly, validation of a melting point is meaningless if the structure is incorrect! A collaboration was initiated with Chemical Abstracts Service, who agreed to provide a collection of several thousand CAS Registry Numbers free of charge to the Wikipedia chemistry community (*44*). A group of Wikipedia volunteers from the Chemicals and Pharmacology WikiProjects then worked through the database provided by CAS and checked the above data fields against Wikipedia chemboxes and drugboxes.

CAS later decided to make the collection fully open to the public on a free CAS Web site (*45*), with links to Wikipedia. The site, called "Common Chemistry," was officially launched in April 2009, and links were soon added to this site from all Wikipedia validated CAS numbers (indicated in the Chembox by a green check mark). Common Chemistry continues to play an important role in the validation exercise for Wikipedia, since now any member of the public who doubts the validity of a CAS number or related structure can (with one click) check with CAS that it is correct. Although Common Chemistry does not cover every chemical compound on Wikipedia, it does indeed cover many of them, including the most common—meaning that the articles receiving the vast majority of hits have been validated.

The problem with a validation process on a freely-editable wiki is that someone can change the information at any time. To meet this challenge, Dr. Dirk Beetstra (Eindhoven University of Technology) has developed a "validation bot" called CheMoBot which logs all edits made to chemical substance pages and compares them against validated versions (*46*). If a validated CAS Number is altered, CheMoBot changes the green check mark to a red X soon afterwards (*47*). The validation process is not completely watertight at present, but it nevertheless provides a strong foundation upon which a broader validation effort can be built in the future.

Other collaborations are under way with IUPAC, ChemSpider (to which two-way links are already in place) and some suppliers of chemical software. Much of this is aimed at improving the reliability of chemistry content on Wikipedia. This supports and enhances the day-to-day work of the WikiProjects in reviewing articles and improving chemistry content.

How to Use Wikipedia as a Chemistry Resource

Many working chemists use Wikipedia as a convenient and extensive online source of information. Chemistry students need to learn how to get the best out

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of Wikipedia while avoiding the pitfalls, just as they should be trained how to use standard chemistry resources, such as SciFinder or Beilstein Crossfire (when these are available). In 2010, an understanding of Wikipedia should be seen as a basic component of information literacy.

One important use for Wikipedia—already well known to students—is to provide a simple introduction to a topic, or a readable overview of a topic. When learning a topic from a textbook, one may get bogged down in the detail; encyclopedias (including Wikipedia) have long been used by students to give a broader view of a subject, often written in a more accessible way (*48*). But the rich internal links of Wikipedia take one further than a print encyclopedia or a textbook: they allow browsing "around" a topic to understand the context of the subject. As philosopher David Weinberger pointed out at Wikimania 2006 (*49*), Wikipedia adds *meaning* to knowledge through its browsability, and this represents a very real advance in how we communicate knowledge.

Related to this is the use of Wikipedia to provide a definition of a particular term. Because of the up-to-date nature of the site, and the tech-savvy editors who make up its community, Wikipedia has become a particularly popular source of definitions on recent technology and terms relating to the Internet. Although this is clearly useful, Wikipedia can attract opinionated people on "hot topics" who may seek to impose their definition on the world; as such, the reader should use such definitions with caution. As with the definition of chemical substance used as an example earlier (*36*), the discussion page will often reveal controversy and debate around such definitions—worth checking if one plans to use the definition in a paper. If a Wikipedia article is to be cited, the user should click on the "Cite this page" link (found under "Toolbox" to the left of the article), as this will ensure that the correct formatting and (usually) a permanent link to the cited article *version* is given.

Another use for Wikipedia is as a portal to the literature on a particular topic. Wikipedia does not claim to be a "reliable source" according to its own definition; it encourages its users to go to primary sources (peer reviewed journal articles and books). However, it has one distinct advantage over a traditional print encyclopedia—much of the source material for its articles is just one click away. (With a Wikipedia article on a broad topic, detailed references may often be found in derivative articles linked from sections within the more general article.) In the last four years, Wikipedia has moved almost completely over to inline referencing, allowing the reader to identify which source was used for which statement. In a well-developed article, these sources come together to give a valuable collection of bibliographic information. Finding suitable reviews and books on a particular subject might take hours of searching in a traditional library, but such sources can often be found in a few seconds on Wikipedia. Specific journal sources are often available online, and many chemistry references use a DOI (Digital Object Identifier (*50*)) which allows the reader to access the abstract and (if available) full text of the article. In this way, the veracity of the Wikipedia article can usually be confirmed by immediately checking the sources, or the user can simply ignore Wikipedia and read the cited literature.

Of course the cited literature used on Wikipedia is by no means comprehensive, and the source articles and examples used can be quite arbitrary

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compared to a peer-reviewed book or review article. Nevertheless, they are often of great value, and they incorporate up-to-date references in a way that no printed resource can ever achieve.

A popular way to use Wikipedia is to find quick little facts, such as the melting point of a substance. Traditionally the chemist might have reached for a *CRC Handbook of Chemistry and Physics*, a *Merck Index*, or even an *Aldrich* catalogue, but for a chemist working at a computer, a Wikipedia search is often faster. Clearly the user needs to trust Wikipedia as a source for such information, though as secondary sources, handbooks and catalogues are imperfect too. My recommendation is that this use of Wikipedia is appropriate for non-critical information, but when the reliability of a piece of information is paramount, or if the information is to be published, other sources should be used to verify the accuracy. Conversely, if information from a handbook is to be used in a publication, a quick check in Wikipedia may be worthwhile in order to confirm the accuracy of the information.

Increasingly Wikipedia is used as a source of images, graphs, charts, etc. I have personally been contacted by working chemists, book authors and documentary film-makers about use of Wikimedia Commons images found in Wikipedia articles, even though the copyright allows these to be freely used without consultation. Our students need to understand how they can use such graphics appropriately in their papers and Powerpoint presentations.

First, it should be understood that the graphic file is reached by directly clicking on the graphic within the article; this brings up an image file on the Wikipedia site, usually with a link to the source file on Wikimedia Commons. The source file usually provides a much higher resolution image than the transcluded file found in the original article. It often provides information on the source ("data in this graph were taken from X") or other useful metadata (such as the date or location of a photograph); most important it provides copyright information. Students should be taught, as part of their training in information literacy, about public domain and copyrights. They need to learn that re-using an image found from a Google search may or may not be legal, and how to correctly re-use files carrying a "Creative Commons" license (used on Wikipedia and other sites such as Flickr).

It is clear, then, that Wikipedia provides a rich resource for our students, in some cases giving a unique and valuable insight into a particular topic. However, they should be trained to know the limitations of Wikipedia, and how to use it appropriately with due regard for reliability and copyright law.

Using Wikipedia for Student Assignments

Students need not be merely passive users of Wikipedia; they can become editors. For this reason, some college faculty assign Wikipedia work as part of their course work (*51*, *52*). This serves several purposes: students learn to write in a collaborative, peer reviewed and high-profile environment, while Wikipedia benefits (in most cases!) from the contributions (*53*).

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Chemistry faculty have taken advantage of this opportunity. At the University of Michigan, graduate students taking courses in 2008-2010 in polymer chemistry or physical organic chemistry were assigned a Wikipedia article to expand or clean up (*54*). At another US university, an undergraduate inorganic chemistry course included a similar assignment (*55*). There were problems found with this type of assignment; often, students uploaded image files without proper attribution or copyright information, and these files were quickly deleted. Aside from this, though, the projects were quite successful, in part because in both cases the instructor worked with both students and the Wikipedia community (often via the chemistry-related WikiProjects) to ensure that citations were included, and that the Wikipedia style guide was followed.

Some guidelines are available at a page on Wikipedia, outside the article-space: http://en.wikipedia.org/wiki/Wikipedia:School_and_university_projects . This page is a good starting point for teachers who plan to have students edit Wikipedia. It lists some active Wikipedians who are interested in serving as facilitators or advisers. The page explains that because Wikipedia has such a high profile, new or badly written articles are often quickly deleted; for this reason, it is suggested that the instructor should consider using another wiki; a chemistry instructor might also examine the possibility of students contributing to VIPEr (*56*) or ChemSpider Synthetic Pages (*57*) where appropriate.

The Wikimedia Foundation guidelines mentioned above (*46*) form part of a series of pages, titled "Assigning Wikipedia articles as coursework to students." The main suggestions are worth summarizing here. Instructors are advised to create a timetable, recruit facilitators, set very specific goals, teach students about the basics of Wikipedia, and consider inviting a public speaker. The instructor should usually suggest specific articles or topics. Suitable projects for university students inexperienced with wiki editing include expanding and adding references to a short article, adding a section to a longer article, or (after checking with the relevant WikiProject) writing a short new article.

If projects of this sort are mismanaged, students and the Wikipedia community come away frustrated and disappointed. But if handled carefully, these projects can be very fulfilling for students, as they see their work on the Web for the whole world to see and use.

Conclusion

Wikipedia has transformed the way knowledge is stored and disseminated, and it has become one of our most useful information resources. Our students have quickly come to value the power of Wikipedia, and it cannot simply be ignored or written off. It is therefore essential that our students learn to use Wikipedia *well*—to learn how it works, and how to get the most from it.

Clearly, students should understand that Wikipedia is fallible, and its content should be treated like any secondary source—with a critical eye. But this is only the start; students can learn *how* to check information they find in Wikipedia, by looking for validated data, links and references. They can use the site to get a simple or quick description of a topic, to "get a second opinion", or they may locate images and diagrams they can legally use in papers or presentations. They may even participate in collaborative writing and contribute to Wikipedia articles. Through all of these experiences, our students will grow as scholars—not just by finding a piece of information, but by understanding what is involved in building and sharing human knowledge.

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Chapter 6

Sceptical Chymists Online

How the Practice, Teaching, and Learning of Science Will Be Affected by Web 2.0

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The current era of science and science education began in the 17th century, made possible by the earlier spread of the printing press. Science remains embedded in its 17th century context, and it is precisely these Gutenberg-era foundations that the Internet is replacing with new ones. The directions in which this is likely to lead science, given the ways in which the Internet is altering our social organizations are discussed.

Déjà Vu All Over Again

Bob's Virtual Community of Scientists

Bob was thrilled about the virtual community of which he was a member. It was a group of scientists with exciting new methods that could be used to investigate myriad questions. They held regular meetings in the old days, but had become scattered across the country. Thankfully, with the help of a social networking system, this "Invisible College" as they styled themselves, was able to keep in contact and to continue honing their methods, sharing results, and arguing about what those results meant. Once a new administration came to power in the capitol, they appealed to the government for recognition, which was granted. Their movement eventually changed the way we all practice, teach, and learn chemistry.

Bob never, not once in his life, laid eyes upon a computer.

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

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Bob's full name was Sir Robert Boyle, today most famous for his gas law. He was also a founding member of the first true scientific society, the Royal Society of London (1660), supported by the new king, Charles II, and was involved in the publication of the *Transactions of the Royal Society* (1665), the world's first true scientific journal. His demonstrations of scientific experiments arguably formed the beginnings of science education. The social networking technology he initially used to keep in touch with his colleagues was the post. While this was an effective way for the small numbers of the Invisible College to communicate, the conversion of this small scientific community to a widespread Royal Society relied on a revolutionary invention: the printing press.

The *Transactions of the Royal Society* made it possible for a scientist to share results with everyone in the world. As Sir Robert Boyle would argue in *The Sceptical Chymist* (*1*), whereas the alchemists had labored in secret, the new "natural philosophers," as the first scientists called themselves, would make their results available to everyone, thereby allowing knowledge to accumulate and for scientists to benefit from one another's work. It enabled, in the words of Clay Shirky, *one-to-many* communication at a distance for the first time in history (*2*). The sharing of results via the printing press, combined with Bacon's experimental method (*3*), gave rise to what we now think of as the Scientific Revolution—the foundation of modern science.

Our own era can be seen as an echo of this period. As Shirky has argued, while the early modern era shifted us from *one-to-one* communication (monks with quill pens) to *one-to-many* communication (the printing press), today we have a similar shift. The Internet is the first medium inherently good at facilitating *many-to-many* communication. Shirky argues that a society with the Internet is a different *kind* of society than a society without the Internet, in the same way that a society with a printing press is a different *kind* of society than a society without a printing press (*4*). Along similar lines, Peter Medawar noted the similarities between the very early 17th century and the very late 20th in his essay "*On The Effecting of All Things Possible*", in which he depicted intellectual culture in transition from one basic paradigm to another (*5–7*).

The reason this all matters for science and science teaching is this: the last such paradigmatic shift literally made possible the Scientific Revolution, and formed the foundation on which its institutions were built. Since information is the warp and weft of science, a fundamental change in the way we share information is not a trivial change to that foundation. The information technologies that came between the printing press and the Internet have either enhanced one-to-one communication (telephone, telegraph) or one-to-many communication (radio, television, phonograph, movie reels), and thus they have changed the character of how we interact (we behave differently over a telephone than in a letter), but not the very nature of that interaction (newspapers and television are both broadcast media). Consequently, these media have had an impact on science and science education without transforming them. If the Internet and attendant technologies such as cellular networks are really the second coming of the printing press, and the original printing press gave us the Scientific Revolution, what will the Internet mean for those of us who practice, teach, and learn science?

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If Web 2.0 Is So Great, Why Aren't We Already Using It?

For all the hype about The Internet, digitally enhanced learning, and Web 2.0 (*8*) one might be forgiven for wondering why the teaching of chemistry has changed so little. We still use textbooks and lectures that look much the same as they did in yesteryear, with the exception of the spread of PowerPoint. Students still do weekly problem sets, and many still fail exams. We've spent countless dollars making our classrooms "smart", but our attempts to use "technology" usually look pretty dumb—the same thing we've always done, but with an electronic device involved. We're chemists. We're supposed to be *good* at technology. Why aren't we any good at this?

We *are* good at technology. What we're bad at is redefining our academic culture. Culture is, by and large, a good thing. It is the vehicle for transmitting hard-earned wisdom about teaching from one generation to the next, which makes it *inherently* resistant to change. It gives us a standard method—when our experiments in teaching fail, we can fall back on that standard. The available technology sets the boundaries to what is *possible* in any given era. Our culture determines what we *actually do* in that space. Technology can change without the culture immediately adapting to it.

Technology Changes First—*Then* Culture

Cultural, social, and economic change will always lag behind technology. If technology is the shape of the container, our culture is the contents. As scientists heavily invested in technology, we like to believe that our culture is a fluid that changes shape to fit the container instantaneously. Culture is more like Jell-O: it may reform to the shape of the container eventually, but isn't going to adapt instantaneously. There was a *two century* gap between the Gutenberg press and the Invisible College. We have already seen one tech bubble resulting from an expectation that the Internet would change our economy faster than it actually could.

Because cultural change comes much more slowly than technology, "Revolution" often seems a poor term. Steven Shapin begins his book on the Scientific Revolution by saying, "There was no such thing as the Scientific Revolution, and this is a book about it." (*9*). This Revolution, too, will happen gradually, more like a tectonic shift, the Earth moving only gradually below our feet. But as Galileo is to have said (apocryphically) during his famous trial in which he denied that the Earth was capable of moving, "*eppur, si muove*"—and yet, it moves.

The 17th Century Foundation

The Tripartite Nature of Science

As scientists, we have three primary functions. The first is the creation of experimental information—the day-to-day experiments that uncover small things about our world. This is an individual job. We record these results like the oldest

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scribes, with a pen. This is a one-to-one transfer, as you produce a single copy. The second function is the dissemination of results. This involves one person at the transmitting end, and the society of scholars on the receiving end. It is a one-to-many transfer, primarily accomplished through publications. The third function is the social construction of understanding. This has received the least attention from scientists and has even been somewhat controversial—it is an aspect of scientific practice that we downplay, as it seems to threaten the "objectivity" of science to leave the ultimate judgment of truth to groups of fallible human beings. Yet every scientist experiences it on a regular basis. When we bounce ideas off of colleagues, when we discuss the meaning of a result at a group meeting, when we engage each other at meetings, we demonstrate that science is, in part, a social process, not the pure work of lone geniuses. We also carry out this process by publication and response, hammering out a consensus over the course of years, as new experiments come to light.

The social nature of science was recognized from the beginning by Robert Boyle as being at the heart of the new experimental method. Shapin and Schaffer chronicled the intense debates between Boyle and the political philosopher Thomas Hobbes in *The Leviathan and the Air Pump* (*10*). Hobbes' model for how knowledge was obtained was, like that of many before him, Euclid. From a handful of indisputable postulates, Euclid developed the whole field of geometry by the tools of logic. What was so supremely attractive to Hobbes was that such results could not be questioned. They fit his totalitarian conception of the state, in which all authority was concentrated absolutely in the hands of the king. As strange as it may seem to us today, Hobbes believed that "civil war flowed from any programme which failed to ensure absolute compulsion." (*11*) The possibility that controversy could linger, that scientists could disagree, that something accepted as true today could be overturned by new evidence tomorrow, was anathema to Hobbes; totalitarianism was preferable to differences of opinion (*12*).

In contrast, Boyle proposed a way of constructing knowledge relying not on individual (and often insufficiently impartial) scientists to determine the ultimate implications of their results, but expecting that scientists would open their findings to the community. The community would, argue about the results, and eventually conclude what they meant. Individuals were free to persist in their own beliefs, but it was only when beliefs in conjunction with the requisite physical evidence became sufficient to convince large swaths of the community that something qualified as new knowledge (*13*). As Bishop Thomas Sprat, the first historian of the Royal Society described it, "It is not I who says this: it is all of us," (*14*) while the 20th century historian of science, Karl Popper wrote, "[S]cience and scientific objectivity do not (and cannot) result from the attempts of an individual scientist to be 'objective', but from the *friendly-hostile co-operation of many scientists*." (*15*)

This new type of information culture, in which ideas were vetted by the scientific society as a whole rather than Hobbes' preferred command authority, was part of a broader cultural shift that occurred in the 17th century, in which the Dutch Republic and England (and then Britain) became what Henri Bergson (*16*) and Karl Popper (*15*) called *Open Societies*. The decentralization of power in these societies took place in theology (limited toleration of individual religious

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conscience), economics (the replacement of controlled manor economies with markets), political power (the development of more representative governments), and military might (large infantry armies replacing an elite cavalry class).

The Tripartite Nature of Science Education

There is a rough symmetry between the modes of communication in science and science education. In education, we also have a one-to-one mode (tutoring and mentoring), a one-to-many mode (lecturing and textbook publishing) and a many-to-many mode (discussion). The first has been highly valued from the pedagogues (personal tutors for children) in ancient Greece to apprenticeships of more modern times. It is the way parents teach their children and the purpose of office hours. The second has existed in the Western tradition since the Medieval universities, in which a lecturer would read a copy of a hand-scribed book, since students could not afford their own copies. Around the turn of the 17th century in the Netherlands and Padua (*17*), large public demonstrations of dissections became a regular part of the medical curriculum. John Seeley Brown has described this as the “Cartesian” method of instruction, after Rene Descartes (*18*). The Cartesian system views *knowledge transfer* as the central aspect of education, from a master to a large number of novices, disseminating information like a printing press: one-to-many. The third facet of learning is social learning. If Cartesian learning emphasizes learning about science, social learning emphasizes how to be a scientist. The latter’s emphasis is on the tacit knowledge in the field—norms, values, aesthetics, conventions, modes of thought, and on participation, as science is a participatory act. The importance of this kind of tacit knowledge was first emphasized by Polyani (*19*, *20*). Students learn different things from each other than they learn from the instructor. Both are immensely valuable, but since the social aspects of science can only be learned in a social group (by definition), this is a critical mode of education for the coming social century.

Why the Social Matters

In the absence of the Internet, the social aspect of science was primarily of interest to sociologists of science. Its role has been important, but it has mostly occurred on a very small scale (the research group, the small, intimate conference). We are now, however, entering into a world in which the capacity of *huge* social networks of science remains to be tapped. Just as proto-scientists disseminated knowledge prior to 1600, but their conception of science was shattered by a transformation in the capacity to disseminate, we engage in the social production of knowledge already—but, as the saying goes, we ain’t seen nothin’ yet.

In the Pre-Modern Era (prior to ca. 1600), science occurred in the context of apprenticeships or single schools, such as Aristotle’s Lyceum. Because there was no means for one-to-many communication, let alone many-to-many communication at a distance, knowledge was created, disseminated, and incorporated locally. The obvious advantages of a face-to-face community of scholars remain today—this is why we have colleges and research universities—but in the pre-modern era, it was *impossible* to collaborate at a distance.

The printing press was therefore a prerequisite to a dispersed scientific community. When the Royal Society was founded, members joined from all over Europe. The communication of results through print became regularized with the *Transactions of the Royal Society*. Results were published for the wider community, but the critical third part of the scientific endeavor, the social incorporation of new knowledge, was carried out in one of two ways—slow interaction through published letters, and face-to-face meetings of the Royal Society. While the pre-modern era, characterized by scribes, had one-to-one distance communication (fine for discovery, but terrible for dissemination and incorporation), and the modern era, characterized by the printing press, had one-to-many distance communication (fine for discovery and dissemination), it was only by gathering at a physical meeting, that the social process of incorporation could occur in real time. The Internet, by contrast, has a native property that Seb Paquet calls, "making group forming ridiculously easy" (*21*). This has the potential to allow scientists to easily form groups to discuss their work and exchange ideas. The scientific community has been waiting for the Internet for four centuries; it just hasn't known what it was missing.

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The Royal Society: The House That Johann Built

Gutenberg's printing press made *possible* the Scientific Revolution without making it *inevitable*; the press existed in many places *other* than northwestern Europe, and existed there for some time without a Scientific Revolution. However, as Elizabeth Eisenstein has argued in her magisterial work, *The Printing Press as an Agent of Change*, it is almost impossible to conceive of a Scientific Revolution in an age of script (*22*).

The first problem of script was that information could not be easily disseminated. Columbus was unaware of the Viking travels to North America and even in the early days of print, Copernicus was unaware of the great trigonometric work *On Triangles* until he was sixty-five years old (which occasioned a major rewrite of *De Revolutionibus*) (*23*). Many discoveries never became common knowledge among scholars.

The second problem was that in an age of script, knowledge degenerated through copying over time. Copernicus as a student had great difficulty accessing Ptolemy's *Almagest* even in corrupted form, copied through the ages in Latin with all the errors in the astronomical tables this introduced, whereas his successor Tycho Brahe could purchase both an original, error-free translation of the *Almagest* from the Greek and Copernicus's modern tables in order to compare them (*24*).

Third, the printing press made it feasible to make science *public*. The rise of a reading public even made it profitable to publish books, manufacture telescopes, and design globes. Bacon condemned the scientists of the past for their secretive, non-cooperative methods, but there had previously been no alternative. In contrast, by the 1660s, Newton's notebooks show that he "devoured books by Boyle and Hooke…took careful notes on the *Philosophical Transactions*…made notes on Galileo's *Dialogues*…and Descartes' *Principles of Philosophy*….as we turn the

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pages of his notebooks we can see his mind leap from summaries of his reading to his own new principles and results." (*25*) This knowledge that Newton really did "stand on the shoulders of giants" should dispel our myth of Newton as a solitary genius. Newton, like all other scientists of his century to now, was a product of Bacon's program of 'open science' (*26*), in which ideas were freely shared and accessible.

Villages, Cathedrals, and Bazaars

The Village People

As hunter-gatherers, we didn't worry about how to organize ourselves. We formed small groups of blood-related people. We probably had very limited forms of social hierarchy, although, even in small tribes, some have *always* lorded it over the others (*27*). I call this mode of organization a *Village*, represented by small groups with strong personal ties. Transactions are handled on the basis of implied reciprocity. Such societies are actually quite good at punishing freeloaders. *Village* organizations still and will always exist: the nuclear family, small church organizations, neighborhood soccer teams, a small online community, and a small business are all *Villages*. We have gradually moved from a world in which everything was organized on *Village* lines, to a world in which two other archetypal patterns have emerged. Their names are taken from Eric Raymond's classic essay *The Cathedral and the Bazaar* (*28*). The *Cathedral* is the hierarchical organization, a metaphor first given by Fred Brooks in *The Mythical Man-Month* (*29*). The large company, the mediaeval Catholic Church, the army, and the political party are all organized in a *Cathedral* mode, named for the top-down way in which the construction of medieval cathedrals was directed.

The *Bazaar* is the sort of chaotic, diffuse-organization mode in which most rules are bottom-up rather than top-down, countless competing forces replace the unifying command structure of the *Cathedral*, and what order there is seems to emerge *as if by an invisible hand*. Representative governments, markets, and the scientific society are all organized by *Bazaar* methods. Notably, *each of these examples* came into being on a large scale in the 17th century, as northwestern Europe developed into Bergson's *Open Society* (*16*), a society undergirded by major *Bazaar* organizations for the first time in European history. The era of the Scientific Revolution was the first age of the *Bazaar*. The second great age of *Bazaar* emergence is our own.

The Cathedral: Taming Complexity through Hierarchy

The complexity of decision making in a group is dependent on the number of two-way communications in the group. A group of one has zero bilateral relationships (I don't need to coordinate with anyone), a group of two has one (challenging enough, as any couple will tell you), and a group of three has three (A↔B, A↔C, and B↔C). The number of pairs equals $(N)*(N-1)/2$, where N is the number of people in the group. As N becomes large, the group's *coordination costs* become proportional to N^2.

This was observed by Fred Brooks in *The Mythical Man-Month* (*29*), in which he explores the paradox that adding software engineers to a late project only makes it later, because the increased coordination costs outweigh the benefits of more people power. Brooks' prescription was a structure in which groups are kept small, with well-defined tasks and responsibilities, built into a hierarchical command structure, so that every work group fits into the master plan.

The *Bazaar*: The Rise of Emergent Order Systems and the Wisdom of Crowds

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The *Bazaar* mode of organization is the most difficult for us to understand and the hardest to believe is actually in operation (we tend to imagine that the *Bazaar* is just a large *Village* or indulge in conspiracy theories that it is run like a *Cathedral* in which ths power structure is invisible or secret). As these responses prevent us from taking advantage of the benefits and power of *Bazaars*, and as we are in an era in which many *Villages* and *Cathedrals* are morphing into *Bazaars*, it is worth understanding the idea of emergent properties—the signature feature of *Bazaar* organization.

Emergent properties are those that are apparent only on a *macroscale*, and that result in a counterintuitive manner from what is going on at the *microscale*. These are different from fractal properties, which are simple extensions of small scale patterns to a larger scale. Natural selection is an example of an emergent property. The microscale activity that gives rise to natural selection is mutation. On a microscale, mutations result in failures of systems. A mutation is *almost* never beneficial to the organism that mutates. However, because *some* mutations are beneficial, mutation has the *large scale* benefit of allowing species to evolve. Similarly, Adam Smith noted that self-interested behavior, often very harmful to very small communities, in very large communities can cause thousands of people to coordinate the providing of each of our daily needs. Chemistry is largely the study of how emergent macro-properties (surface tension, crystallization, conductivity) result from micro-properties (hydrogen bonding, Coulomb's Law, and delocalized bonding, respectively).

Walter Russell Mead describes this idea that, if the system is under the right conditions and rules, a benevolent order can spontaneously emerge, "The Golden Meme (*30*)". Bacon, drawing on his appreciation of the way in which the grand principles of English Common Law had emerged from small, narrow cases, built his conception of the scientific method, in which grand theories would eventually grow from many simple experiments. In spontaneously ordered systems, error, sometimes spectacular error, be it in law, science, the market, or biological evolution, is not only a consistent handmaiden of the development of new systems, but a *vital* mechanism of correction. Boyle, in articulating science as an *experimental* process through which theories emerge, built a system in which we learn through error. Scientific society was, from its inception, a *Bazaar*. In contrast, in Hobbes' *Cathedral*, trial and error could not be countenanced, because error is deadly.

It is only relatively recently that we have come to appreciate how powerful *Bazaars* can be. James Surowiecki in "The Wisdom of Crowds" (*31*), gives countless examples, ranging from science to software, trying to explain the phenomenon that while crowds can sometimes be foolish, such as the herd-like stampede of a market crash, there are other times when the crowd is dramatically smarter than the individuals of which it is comprised. Glenn Reynolds argues that in the Internet Age, we should organize "Like a pack, not a herd," (*32*) suggesting that we can act as independent, yet coordinated actors in pursuit of a goal like a dog pack. But how do we get a *Bazaar* to *act* like a pack and not a herd? Surowiecki suggests at least a partial answer: the Wisdom of Crowds requires the presence of diverse opinions and convictions, deeply held within the system. When too many people working on anything succumb to "group think", the group ceases to be self-correcting, and becomes self-reinforcing. This creates a paradox: the Wise Crowd is smarter than the individual, but the Wise Crowd only functions because it is comprised largely of individuals who think they are smarter than the Wise Crowd. Only these independent thinkers provide the diverse ideas out of which the best emerge. The implications of this for science, particularly as science becomes more *Bazaar*-like, are enormous. We must cherish our heretics. The enduring disagreement among scientists that Hobbes thought was our Achilles' heel is actually our greatest strength. We must face head-on the paradox that as a scientific consensus forms, it becomes more likely to be correct, but the importance of listening to the dissenting voices *increases* as the probability of the validity of their dissent *decreases* (*33*). Only by refusing to let Newtonian mechanics become sacred truth could we adopt quantum mechanics.

Hayek's Knowledge Problem and the Long Tail

Hayek first explained another key advantage of the *Bazaar*: it is far better at managing the *information problem* that plagues *Cathedrals* (*34*). The CEO doesn't know what's going on at the widget factory; the general doesn't know that a battalion just discovered the enemy reserve; Pope Leo X didn't know Martin Luther was about to tack 95 theses to the door. John Seeley Brown once asked of Hewlett-Packard, "Imagine if HP knew everything that HP knows." One person can never know all that is going on in a large organization. Furthermore, much of this information is tacit - the possessors of the information often don't even know that they know it or that it's important.

Bazaar structures, in contrast, are very good at mustering tacit knowledge, because the organization is more flexible. If the information *problem* is that the important tacit knowledge is widely distributed, a distributed communication structure will best harness it. One key advantage of the *Bazaar* structure is that an individual doesn't have to be *assigned* to a task in order to contribute to it in a small way. In a *Cathedral* organization, I would never be *hired* to write or edit a Wikipedia entry on the Glorious Revolution (a 1688 event that has nothing to do with chemistry). Yet, I recently discovered an error, and corrected it in seconds. That flexibility allows those with useful knowledge to be able to contribute at *any* level. This is one example of the phenomenon described by Chris Anderson in *The Long Tail* (*35*). The useful knowledge on a given subject is not evenly distributed throughout the population, but is instead distributed in a power law. The one shown in Figure 1 arbitrarily uses the formula $y = 1/x$. Those who

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know the most about the Glorious Revolution are on the left. One could imagine assigning the ten most knowledgeable people to the job of writing the article. The question then becomes: even if the other ninety people know little, what is the sum total of their knowledge? For this particular power law, 56% of the knowledge is held by the top ten experts, and 44% by the ninety amateurs. If one extends this graph to a community of 10,000, such that the least expert member knows 1/10,000 of what the most knowledgeable member knows, then our "top ten" possess 30% of the total knowledge, and the amateurs possess 70%.

Different forms of knowledge obey different power law distributions: some are very concentrated, and thus have a very fast decay (such as expertise in brain surgery), and some are very dispersed and thus decay slowly, with a great deal of area under the "long tail" of the curve (such as expertise in photography). "Science" and "teaching science" are more like photography than brain surgery in that the *useful knowledge* is very dispersed. Even if you have the top ten experts in a given field working on a problem (say, those within a research group), there is an enormous amount of information potentially useful to the project that is possessed by others in the society under the long tail.

So When Do We Use What?

Villages are simply the best structures for anything small. The balance between *Cathedrals* and *Bazaars* is shifting, but some *Cathedrals* will certainly remain. The primary factors in the shifting equilibrium are:

(1) **Cash to the Cathedral.** Projects involving large outlays of capital will favor traditional *Cathedral* organization. Large amounts of cash require large amounts of accountability, and the "who answers to whom" structure of a *Cathedral* is very important for that purpose. Those *Cathedrals* that are the most vulnerable in this category are those that *used* to require cash outlays, but no longer do, such as publication.

(2) **Bazaars Aggregate Dispersed Knowledge.** Projects with highly *concentrated* knowledge will favor more traditional *Cathedral* organization, whereas dispersed knowledge will benefit from *Bazaar* organization. Because it catalogs all human knowledge, Wikipedia is best created by a dispersed *Bazaar*, yet the control systems for the Boeing 787 should probably remain within a highly competent professional hierarchy. The most vulnerable *Cathedrals* here are those that rely on dispersed knowledge, but traditionally have existed within *Cathedral* structures because the tools did not previously exist for an efficient *Bazaar*, such as textbook authorship.

(3) **Falling Coordination Costs.** Ronald Coase argued that given the advantages of *Bazaar*-style free markets, that the primary reason why one created *Cathedral*-like corporations at all was to *coordinate* the workers to work on a large project—to act as middle men in a market (*36*). In many contexts, the Internet is slashing these coordination costs, making it far easier for individuals to organize themselves without the intermediacy of *Cathedral* organizations. Anywhere an existing

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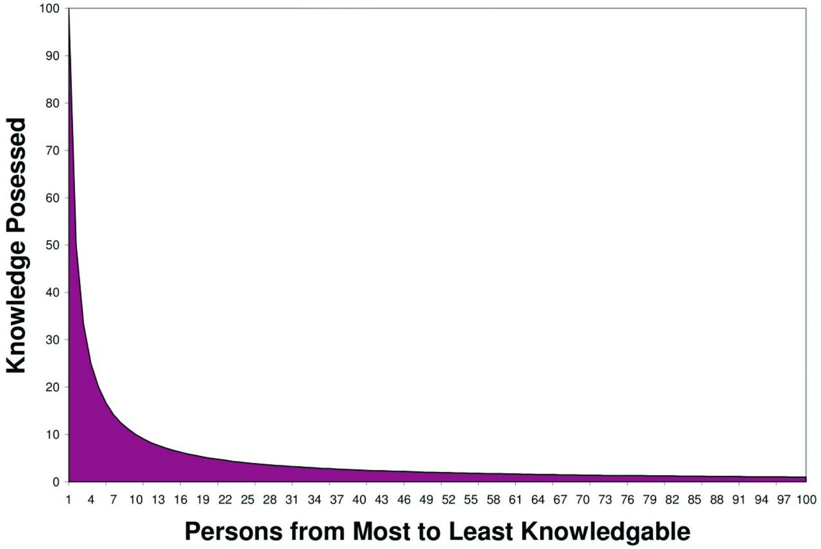

Figure 1. A Power Law Distribution of Useful Knowledge

> *Cathedral* has as its sole justification the management of coordination, such as the way that job ads are carried by print media, that *Cathedral* is susceptible to challenge from a *Bazaar*

Science Then and Now

Science Practice

Science before the 17th century was always carried out in *Village* mode, with Aristotle's Lyceum being a classic example. The scientific community was small, and held together with strong personal ties, in one physical locale. The technological and social changes in the 17th century, resulting from the ease with which results could be published and distributed, made possible the rise of a *Bazaar* of scientists, albeit one small enough to have many *Village* characteristics.

In the 19th century, Justus von Liebig's laboratory developed something of a *Cathedral* structure (just as the printing press created a great shift toward *Bazaars*, the Industrial Revolution occasioned a smaller backslide toward *Cathedrals*). Von Liebig invented the modern PhD laboratory, in which a group of graduate students worked for a single professor. The hierarchical structure of science, even in the German system remained fairly open, however. More importantly, the rise of large scale chemical *industry*, with its need for large capital investments and accountability for their expenditures, drew much of chemistry behind the *Cathedral* walls. Chemistry lags behind both biology and physics in the practice of open publishing, due in part to the need for and culture of corporate protection of patentable research (*37*). During the 20th century, the ACS (American Chemical Society) *Cathedrals* of the field were erected: the ACS publication system, the ACS as a political-professional organization, and the ACS as a meeting convener. In the post WWII era, the National Science Foundation and National Institutes of Health have become mainstays of research science. The ACS and the funding agencies are largely *Cathedrals* that yet retain a key *Bazaar* feature: the involvement of community members in the governance, review and panel process.

Science Teaching and Learning

The practice of *teaching* science, in contrast to *doing* science, has become much more institutionalized into the *Cathedral*. Beginning with the foundation of large lecture halls such as the anatomical theater, science education has largely followed a Cartesian model, with all the peripheral students connected to the central professor. The structure of courses, departments, and universities is also very hierarchical. Everyone has their job to do and their reporting structure. As the population of students has grown, the scale of courses has tended to make them less like *Villages* and more like *Cathedrals*. Some institutions have managed to foster a *Village* atmosphere amongst students doing homework together in the dorms, and this remains the ideal of most tutor systems and liberal arts colleges. There has been, however, very little attempt to create a *Bazaar*, something which is large and geographically dispersed, and can tap the Long Tail of knowledge.

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The Third Millennium and *Bazaars*

The scribal book is a *Village* phenomenon. It can be read and shared amongst a small group of people, and cannot be copied to scale. The same is true of the individual experimental scientist working at the bench, and recording the work in a book. The printed book or journal is a *Cathedral* phenomenon, produced at a capitalized center, and distributed to the masses. The Internet and all its works is a *Bazaar* phenomenon, as is the social construction of knowledge by scientists, because the analysis of a result, and the use of that result to suggest new experiments is a process that can benefit from the knowledge base of the whole community. We are entering the Millennium of the *Bazaar* as the Internet destroys coordination costs. The Open Source Movement, the inspiration for *The Cathedral and the Bazaar*, has been a bellwether because its participants were the original Internet natives, yet the ideals of open source and science are the same: “In science, one’s private property is established by giving its substance away.” (*38*)

Two caveats need to be held firmly in mind: the transition will be *slow* and it will be *incomplete*. A century from now, the world will be full of *Villages* and *Cathedrals*. But everywhere the emergence of a *Bazaar* is being held up only by a not-too-complex failure to coordinate, and everywhere that widely dispersed knowledge is necessary to a job that a *Cathedral* is now doing, we should be expecting change.

Science Belongs in the Bazaar

Why has scientific practice remained largely rooted in the *Bazaar*? The answer lies in the irreplaceable nature of the social component of science. Even in Boyle's day, there *could be* no science without a scientific society. Interpretation of results and the assessment that a point had been proven were *always* group phenomena, which both removed the dangers of bias of the individual researcher and integrated the new findings of a researcher with everyone *else's* knowledge. Scientists are, by nature, infovores. We are traffickers in knowledge. Because of this, Hayek's "knowledge problem"—the fact that useful knowledge is highly distributed, has always been one of the biggest considerations in science. Not only has it always been critical to distribute results, but also to hear criticism and ideas from the entire scientific society. Very often, the best ideas do not come from one's own research group, or even groups very closely related, but rather from researchers more distant. In a *Cathedral* structure, in which scientists only interacted with those in their "subdivision", every researcher would be cut off from the enormous body of knowledge of all other researchers. *Bazaars* attack the knowledge problem by letting anyone talk to anyone. A remarkably successful example of a *Cathedral* using *Bazaar* architecture is Innocentive (*39*, *40*), a spin-off of Eli Lilly that posts challenges to the Internet with cash prizes for marketable answers.

It is the anyone-to-anyone pattern that is set to explode in the coming century. Just as the printing press made it possible to share results with the world, the Internet makes it possible to share your discussion. The most common form of collaboration between universities right now occurs hierarchically. Group members collaborate and interact with their PI, and PIs interact with one another in collaborative discussions. However, *graduate students* at different institutions rarely have such conversations with each other without going through their PIs. Fear of being scooped has been the first factor inhibiting a radical openness in our research culture. The other factor has been that the technological barrier to student-student contact has been high enough to discourage facile conversation. This is rapidly changing as students across the country communicate in real time. Most scientific collaboration in the 21st century will *not involve PIs*, nor will it be supported by NSF funding, nor will it even be done necessarily with PI knowledge. It will primarily be done, informally, through a network of friends of friends of friends, helping each other out in their research *because that's what friends do*. It should be noted that this will make high quality graduate students *more* valuable, and will favor PIs who motivate and manage well at the expense of brilliant petty tyrants.

How will we then prevent scoops? How will we assign "credit" for work that is so dispersed? How will we evaluate people for tenure? Their next grant? I think the answer is that we need to remember that the Internet is an improved printing press. To *publ*ish means to make *publ*ic. Once it has gone online, *it has been published*. We have traditionally associated peer review with publication (the second part of the experiment-publish-discuss trio). This is a mistake: peer review is a part of the *discussion* of science, and the model we will gradually shift to will look rather different. Our current practice decides, on the basis of

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peer review *whether experimental results* should be shared, and it will shift to determining whether the *analysis of published results* is correct. Furthermore, our current institutional structure that locks researchers into a *Cathedral* mode of publishing inhibits the shift to open science. We must envision new funding structures that allow for much broader and easier access to scientific information throughout our community.

Formal 2-4 person peer review will almost certainly be replaced with what Eric Raymond calls "massively parallel peer review": post-publication review of materials by the community at large (*41*). The Open Source community went to this model because it did a *more effective job* of finding errors and improving the work, and that it was the only method that scaled to as large a project as Linux. The growth of science to a truly global phenomenon will greatly increase the number of such reviewers, making real the claim of Raymond that, "given enough bugs, all problems are shallow" (*42*). As Shirky describes the shift, we will shift from "filter then publish" to "publish then filter" (*2*). It must, however, be stressed that this "revolution" will play out over a century, not a decade, and that we lack the filters today to sort the good from the bad in the scientific commons.

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If We Practice Like Boyle, Why Do We Teach Like Hobbes?

If science inherently belongs in the *Bazaar*, and scientific teaching and learning has an incredibly important many-to-many component, why have we gotten away with a *Cathedral* mode of teaching for so long, and what is likely to change as coordination costs fall? In answer to the first question, I would argue first that the teaching methods that have focused on the use of non-*Cathedral* methods are actually attempts to make the classroom more like a *Village* than a *Bazaar*. There is a peer-to-peer aspect to this teaching and it is valuable for teaching the methods of the social construction of knowledge: how to work with others that have different approaches, how to engage in give-and-take, how to learn from one another, and how to communicate science to their peers. These are all *Bazaar* skills, which can be taught in a *Village* setting. The possibility for teaching that accesses something larger, a true global *Bazaar*, simply has not existed until now. There has always been a balance between the "Cartesian" mode of teaching (learning is information transfer) and "Social" teaching (learning is learning to practice in the field). Cartesian learning is teaching like a printing press: one to many; from the authority to the masses. This was Hobbes' ideal for education, not Boyle's, where understanding comes from discussion and the free exchange of ideas. Discussion-based learning is the mode native to the Internet. In a pre-Internet era, the information was so hard to come by that information transfer was extremely important. While its *relative* importance will decrease, it will remain important. The rise of the printing press did not supplant the need to teach laboratory technique just because it made possible the learning of cumulative knowledge in the field through lectures and books, and the rise of the Internet will not eliminate the need for Cartesian knowledge transfer.

The Internet *does* remove the *scarcity* of information that made an expensive textbook or an expensive professor's lecture a pearl of great price. To *publi*sh no longer requires a large capital outlay. Increasingly, excellent lectures on virtually

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any topic are available online, and this is in its infancy. To try to charge students exorbitant prices for textbooks and lectures in the late 21st century will seem as ridiculous to our latter-day students as it would have seemed for a 17th century professor to insist that students pay a monk to scribe and illuminate a copy of Copernicus' *De Revolutionibus* for each of them. Our focus on distribution of knowledge was predicated on the notions that the content of the course was the most important part, and that the students couldn't find the content themselves. If the *content* becomes much more accessible, we will either, as educators, have to decide whether we are willing to be paid considerably less, since that part of our job has become much less valuable (the option currently being pursued by the record companies and newspaper industry), or we will need to shift the nature of our training to emphasize social learning—*training* students to use the *Bazaar* in a professional context.

We have always done this, but have largely disguised it; we need to make it our explicit focus. In 2008, Chris Avenir, a first-year student at Ryerson University in Toronto, was charged with 147 cases of academic dishonesty for starting a Facebook group as a place for discussion and the posting and solutions of general chemistry homework for his class (*43*, *44*). As far as he was concerned, this was a study group. The difference here was that with 147 students, most of the students would not participate in the active solution of each problem. This is a typical power law *Bazaar* effect: a few work, the rest freeload. If your goal is to write a kernel for Linux, this is fine. Taking advantage of the *Bazaar* is a more efficient way of accomplishing the goal, *i.e.* getting the homework done. The problem, which Chris Avenir didn't appreciate and his professor probably never explained, was that the answers were never the point. The point was always the process of working through the problems. The *accusation* was even grounded in these terms: that he had made available the *answers* that other people had not obtained themselves. The answers were held up as the object of desire, and it was their *theft* that was the underlying crime. The point was always thus: the answers are useless. The instructor already knew the answers. The goal of the homework assignment was to learn problem solving skills. This needs to become the *explicit* goal of our education.

More than in the Gutenberg era, the Internet era will require our students to work in various different fields and careers, many of which have not been invented. Our students will not return to college for job training. We therefore need to shift the emphasis from the *current* equilibrium between job training and training students to self-teach toward a new equilibrium in which self-teaching is more heavily emphasized. An early example of this is to be found in *Disrupting Class*, in which the authors argue for a radical decentralization and emphasis on self-teaching at the high school level (*45*). Our job in managing this transition is made more difficult by the organization of courses by content. We don't call general chemistry "basic quantitative problem solving", even though that is far more important for even our chemistry students than pV = nRT. Cory Doctorow perhaps put it best:

> Content isn't king. If I sent you to a desert island and gave you the choice of taking your friends or your movies, you'd choose your friends—if

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> you chose the movies, we'd call you a sociopath. Conversation is king. Content is just something to talk about (*46*).

We could replace conversation with "problem solving", "teaching one another", or "learning to collaborate as a chemist". But pV=nRT? *That's* just something to practice on. That's on Wikipedia now. This plays to our greatest strengths as a scientific society; we should not fear it. Many educational systems do a better job of teaching lab techniques and many do a better job of teaching content. Look at American exam scores. But in problem solving, teaching each other, and the collaborative practice of chemistry, we have a comparative advantage. We should embrace it.

We will have to. A *Cathedral* mode of teaching was fine for students raised on broadcast media: the book, the pamphlet, the radio, the television, the LP, the CD. Today's medium is participatory. Web 2.0 is *interactive*. Our students will literally not sit still for a sermon in the *Cathedral*, so we'd better learn how to teach in the noisy *Bazaar*. Our students will grow up in a many-to-many world; they won't stand for one-to-many education. For students who grew up being fed one-to-many, non-participatory media, Hobbsean education seemed natural. To the coming generations of students it will seem as quaint as alchemy.

Sceptical Chymists Online—The Global Society for the Improvement of Natural Knowledge

It is notoriously difficult to make predictions about the future—doubly so in the midst of a revolution. One comforting fact is that this will be a slow revolution. We have time for what FDR called "bold, persistent experimentation". It will play out over a century, as the shock waves of the printing press played out over 200 years. We should focus our experimentation in the *directions* suggested by our predecessors in the 17th century. Science and science education underwent a shift in the 17th century from a *Village* mode to a mode that was part *Village*, part *Cathedral*, part *Bazaar*. Our current shift will be one that radically favors the *Bazaar* mode, especially where the *Villages* and *Cathedrals* are most vulnerable. This can direct our experimentation, but will not give us solutions. I therefore close with a final exhortation. If we are finally completing Boyle's program for what it is to be Sceptical Chymists, then we should take his argument to heart that it is critical to share the results of our *failed* experiments. When print was dear, it was permissible for us to only make public our great success stories. After all, if you can only share a small percentage of what you learn, you pick the gold, not the dross. Now that publication is free, as scientists and science educators, this means a radical new openness. It means sharing our *daily* data with the world, through open notebooks for practitioners, and what we have elsewhere called *Visible Teaching* for educators: sharing the day-to-day results of our experiments in the classroom (*47*).

The 17th century gave rise to the first great *Bazaars*: large-scale representative government, large-scale marketplaces, and the Commonwealth of Learning, the last including science itself. It is beyond our imagination to know what changes the 21st century will bring, but by looking at the past, we can glimpse the rough outlines of our future. As Twain allegedly said: history does not repeat itself, but it rhymes.

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Chapter 7

Creating and Using a Personalized Information Management System

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The current broad array of social networking tools has created numerous new methods of processing and organizing information that are customizable for each individual. Information collected through RSS (Real Simple Syndication) aggregators may also be organized through social tagging tools such as Delicious or Connotea. The collaborative process of shaping a document through a wiki reflects the iterative process of writing as well as presenting an impartial tool for attributing participation in a group project. Back channel communication systems such as Twitter or Google Jockeys potentially take advantage of students' own messaging habits to enhance student engagement. Many of these tools have already been used effectively in the classroom, and training our students to use these applications efficiently is an important investment in their ability to manage the continuous proliferation of information.

I. Introduction

There is a long-standing tension between the ability of scientists to create new information and the ability to organize that information. As long ago as 1945, Vannevar Bush, Director of the U.S. Office of Scientific Research and Development during World War II, published an article entitled, "As We May Think" that discussed the problem of information overload and proposed the creation of a new device, called the memex (*1*), which would make information more organized and accessible on a desktop. This proposal was eventually the

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.; ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

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inspiration for the development of many components that became modern desktop computing.

In a similar vein, Derek de Solla Price, in a chapter entitled "The Diseases of Science" pointed out that the exponential growth in the number of science journals led to the creation of abstracting journals (*2*). Abstracting journals, in turn, showed a similar exponential growth in numbers. By 1950, the number of abstracting journals had reached 300, which de Solla Price considered to be the point at which he expected the development of, ". . . some process of electronic sorting of abstracts as a means of coping with the rising flood of literature." John Willinsky suggests that there are currently about 50,000 scientific and scholarly journals published world wide but admits that the number is only an estimate (*3*).

Not only has the scientific community failed to solve the problem of information overload that was identified by these authors, it is quite probable that the digitization of information has made the problem much worse. Journals, including many that are online, continue to proliferate; new forms of publication are being created; and new forms of communication, like blogs, wikis, and Web sites have further complicated the attempts to keep up with the latest scientific information. Fortunately, the digital revolution is also providing a potential solution. The prediction by de Solla Price that electronic organization of information would appear has finally proven true, although it took much longer to occur that he might have expected.

There is an obvious need for better ways for researchers and students to deal with information overload. Web 2.0 and social networking programs that are already widely available will alert readers to new developments in their field of interest, allow more efficient organization and access to personal information databases, and facilitate improved collaboration. The 2010 Horizon Report predicts an increasing interest in just-in-time, alternate, or non-formal avenues of education, such as online learning, mentoring and independent study (*4*). This suggests that scientists will spend as much time learning informally as they do in formal classes, and so there is a need for a support system that will facilitate lifelong, individual learning. Thus, to the extent possible, solutions should be free and, if possible, not tied to any proprietary restrictions. It would be futile to teach the use of a system that will no longer be available after graduation or upon moving to a new job.

This discussion will focus primarily upon ways to introduce these concepts to undergraduate chemistry students, but it is apparent that these techniques will not be limited to students and can be useful to graduates. Some readers may recognize that the above description is similar to the idea of a Personal Learning Environment (PLE), which has been widely discussed (*5*). The authors of this chapter have avoided using this term since there seems to be little agreement on the specific components of a PLE, and many of the models suggested appear so complicated as to discourage attempts to integrate them into the already crowded chemistry curriculum.

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II. Information Collection: Really Simple Syndication (RSS)

It is generally accepted that an effective undergraduate chemistry program should introduce students to using the chemical literature. Today, most students learn to use *Chemical Abstracts* either with a manual search or, more likely, using an online service, such as SciFinder Scholar (*6*). In addition, they may learn to use a World Wide Web search engine, like Google or Bing, which will allow them to search for information on the Web. These methods are basic, but neither is ideal for keeping up with the recent literature. This task has always been more difficult to teach. Professional chemists might form a journal club or else dedicate an afternoon to reading current journals in the library, but it is often difficult to convince students to read the current literature. One possible approach to teaching current literature awareness is to use RSS feeds.

RSS (Really Simple Syndication) connects a user to a Web site in order to inform the user whenever the site has been updated. There are several variations of the RSS protocol, but all of them function in a similar fashion. As Hammond *et. al* explain (*7*), "RSS is not any formal standard but is rather a tribe of competing 'street' standards." Once a subscription has been set up, the subscriber is automatically notified of new material very soon after the site has been changed. In addition to directly accessing a Web site, such as an online journal or Web page, it is also possible to set up an RSS for a Google search so that the subscriber will be informed whenever there is new material from that search. RSS feeds provide a simple way to deliver very up-to-date chemical information to a student or faculty member's computer.

The key component for this process that subscribes to RSS feeds is the RSS aggregator, sometimes called a newsfeed aggregator or feed reader. As the name implies, the RSS aggregator organizes the various RSS feeds onto one or two Web pages, depending on how many feeds are being tracked, creating a constantly updated personal information space that the user may access at will. There are a number of RSS aggregators available, most of which are free for downloading.

Aggregators are available that work on all of the common operating systems, including Unix and Linux. Aggregators may reside on a specific World Wide Web site, such as NetVibes or FeedDemon; they may be a feature of one of the common Web browsers, or they may be connected to a search engine, like Google. When Pence and Pence (*8*) reported on the use of RSS in the classroom, they suggested that they preferred NetVibes (*9*). Pence and Pence explained their criteria for this selection by saying that NetVibes could be used on Mac and PC computers, worked with a variety of Web browsers, and was free. There are now several other popular aggregators which fulfill these requirements, such as Bloglines, Google, or MyYahoo and which may be more convenient for setting up feeds (as noted below).

Setting up a feed is usually easy. Most search engines display one of the symbols in Figure 1 to indicate that a site has an RSS feed, and it is only necessary to click on the symbol to establish a feed. Unfortunately, browsers limit the number of selections possible. When using the Mozilla browser, the aggregator options are Bloglines, MyYahoo!, or Google. If one is using a recent version of Internet Explorer, the easiest option for setting up a feed is to use the Internet Explorer

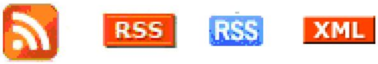

Figure 1. Symbols that indicate availability of an RSS feed.

aggregator. Probably the most convenient choice is to use the Mozilla browser and either Bloglines, MyYahoo!, or Google. Any of these three should be quite adequate.

The method that gives the greatest flexibility in choosing an aggregator is to copy the feed address and paste it into any aggregator of choice. Clicking on the RSS feed symbol will go to a page with the feed on the address line. The American Chemical Society provides a Web page (*10*) that links to over 40 RSS feeds for its journals and *C&E News* (N.B. The URL for this page has changed since the article by Pence and Pence.). One significant limitation to using RSS feeds is that they often cover only a limited subset of the articles in a given journal. This problem can be solved by linking a traditional Web search on a specific topic to an RSS feed, so that the aggregator will show the update every time a new result is found.

The project described by Pence and Pence (*8*) was intended to stimulate student engagement with the most current literature, since although some textbooks reference journal articles as part of homework questions, the tendency to favor classical examples and the time delay between writing and publishing a textbook combine to emphasize slightly older research. In contrast, focusing on articles highlighted by an RSS feed precludes inclusion of anything but the most recent literature. In the project framework, the students were each required to set up an RSS feed from a specific journal in the discipline of the class. The journal was selected so that the students would all have full electronic access to the content, which is essential to make effective use of RSS feeds. On each of 10 homework assignments, several questions were included requiring the students to access several articles from the latest RSS feed in order to craft a response.

A series of focused homework questions, such as those described in this project, breaks an article into smaller pieces and makes it easier to understand. Two basic steps are required to create and use an RSS desktop feed: choosing a reader to receive and organize the newsfeeds, and then connecting selected RSS feeds to the reader. Ultimately however, RSS may have limited application in the classroom. The project had the desired effect of incrementally training the students to read the primary literature and demonstrating that even cutting edge research is based on the fundamental principles of a field, but since the students could access the papers via the citation, the RSS feed itself was not essential for the students to complete their assignments.

When considering the application of a social networking tool to a class, it is essential to consider exactly how the students use a given tool. Trying to force the students to use a tool in a way that does not come naturally to them is counter productive and does not generally result in successful outcomes. RSS feeds will remain invaluable for organizing a vast quantity of incoming information, and students should certainly be exposed to this resource, but a classroom application of this tool for which it is the most direct and natural method for students to complete an assignment has yet to be developed.

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A potential peripheral coursework application of RSS for faculty and students is in monitoring blogs, especially those that students create in response to assignments. The professor can monitor what student work has been submitted and focus his or her attention exclusively on new work, but the set of homework assignments described above and the monitoring of student work submission has greater utility for the professor than for the students. Students may take advantage of RSS to monitor the availability of course content posted on the Web if a feed is set up or to keep abreast of contributions to a class discussion board, but that use is more of a convenience than a skill essential to any course.

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III. Information Organization: Social Tagging

Traditionally, information classification depends upon hierarchical schemes, like the Dewey Decimal system or Library of Congress Classification (LCC); however, some people apparently feel that so much information is becoming available so rapidly on the World Wide Web that cataloging specialists can no longer keep up. David Weinberger argues (*11*) that moving from paper to electrons for knowledge storage changes the rules. Things made of atoms, such as a card catalog or an abstract in *Chemical Abstracts*, are physically limited in the accessibility. Digital classification using electrons makes it inexpensive to have multiple access points to the information. For example, think of how many different search terms can lead to the same resource on the World Wide Web. Weinberg suggests that the best way to classify information may be to just ignore hierarchies, classify everything as miscellaneous, and allow a search engine to sort out what is needed.

An alternative nonhierarchical classification model, called social tagging, has become very popular. Here the users label information by creating social tags (i.e. keywords). Many of the most popular Web sites, such as YouTube, Flickr, and Amazon use some form of user-generated social tagging. Social tagging also has limitations. The idea is too new to have developed widely accepted ground rules. Social tags often have no context, so an image of a rabbit with its mouth open is just as likely to be tagged with the particular rabbit's name as it is with something totally unexpected, like opera. This is enough to give heartburn to the creator of the Dewey Decimal System, Melvil Dewey. The collaborative process of creating and managing tags to annotate and categorize Web content creates what are called folksonomies, that is, a classification system based on user-generated tags.

Social tagging seems to have become widely accepted, even if librarians may be uncomfortable with the practice (*12*), It seems probable for the present that social tagging and professional subject cataloguing, such as occurs in the library, will coexist even if the relationship is uncomfortable. It is probably too late to impose any general order on the creation of social tags, but at least each individual should decide upon some personal ground rules.

This discussion will focus on two social tagging sites, Delicious and Connotea. Delicious is one of the most popular sites for tagging general articles, whereas Connotea is created by scientists for scientists. Despite this difference in original purpose, these sites show many features in common, partly because the

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creators of Connotea, the Nature Publishing Group, consciously used Delicious as a model when they created Connotea in 2004. Both sites are online and are accessible from any Mac or PC computer, and both sites allow the installation of browser buttons that allows the user to save a site more easily. When a site is saved that has been tagged by previous users, both Connotea and Delicious recommend tags for a reference based on previous user tags. There is some evidence (*13*) that suggests tags used by others produce a convergence to a common set of tags, minimizing one of the common problems with social tagging.

One significant advantage of Connotea is that it allows the use of DOIs to identify an article or Web page. A Digital Object Identifier (or DOI®) is a way to identify an object, such as an article or a Web page, in the digital environment. Even if the location of the object changes, the DOI remains constant and so provides a way to locate the object. According to the International DOI Foundation (*14*), "The DOI System provides a framework for persistent identification, managing intellectual content, managing metadata, linking customers with content suppliers, facilitating electronic commerce, and enabling automated management of media." In practice, this identifier means that as long as a user has access to a database that contains the article, he or she can often go directly to that reference, rather than clicking through the various levels of a search. In addition, Connotea allows a user to see other items that have tags similar to those used on articles of interest to the reader and also to connect with other users who have used similar tags. This produces community-driven recommendations which can sometimes be very valuable. Connotea will also use the URL for a Web page or journal article and fill in the necessary information, i.e. volume number, pages, etc., to create a complete reference.

On the other hand, sites like Connotea seem to have more trouble with spam than Delicious. In his blog, Kent Anderson (*15*) suggests that this problem has become serious enough that to affect Connotea. Anderson contacted a representative of Connotea, who agreed that spam reduced the utility of Connotea as a site for ranking science and also created artificially high usage levels that could degrade the system response. Some users feel that the tagging process is inherently less efficient than searching a file of personal pdfs that an individual has saved. Of course, this eliminates the possibility of community-driven recommendations, which is arguably a major reason for using social tagging sites.

Social tagging and Delicious have proven to have a powerful two-fold impact educationally (*16*). First, it is highly desirable that before a Web site is tagged by a student, the student is required to evaluate the Web site for quality. Although there is no standard rubric for such evaluations, looking for how recently a site was updated, whether or not the author is qualified to report on the topic or whether an author's name appears are all common features. The organizational structure, grammatical correctness, and viability of the links are indicators of quality. It is valuable to instill in students the idea that evaluation essential so that they do not assume that all electronic information is equally reliable.

Two other qualities of a Web site are closely linked. First, it is important to evaluate the purpose of a Web site and the information on it. A Web site intended to inform about a topic will have a different perspective from one intended to persuade or to comment. Determining the purpose of a Web site

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assists in establishing the second related quality, which is the bias of the site. When addressing the bias of a site, it is wise to remember two slogans from the old TV series, *The X Files*. “The Truth is out there,” and, “Trust no one.” If asked whether a Web site is biased or unbiased, it is easy to leap to the conclusion that a Web site is unbiased, but realistically, that actually means that the bias in the information is acceptable for the intended use or matches that of the user. Political bias is often easy to spot, but there are biases that may be incorporated without intentionally omitting or shaping the available data.

A site such as Terrific Science (*17*) may be completely accurate, but is biased toward presenting information at a child’s level. Even a site such as scorecard.org (*18*), which accesses the Toxic Release Inventory data directly, is biased because of the bias inherent in the original data and because the site has apparently not been updated recently. It is not that the data were intentionally edited, but for example, small quantity waste generators are not required to report their emissions, and there are chemicals such as uranium that are not on the list of required reported releases. The opportunity to discuss both intentional and unintentional bias of Web sites is invaluable for students, who tend to use all data and information obtained from Internet sources without evaluating or assessing it.

Although it is possible for individuals to share bookmarks, as noted previously, the most straightforward approach to using a social tagging utility such as Delicious in the classroom is to have the students and professor share a joint account with the same username and password (*16*). This account should be separate from personal accounts since everyone will have access. Several different models of using Delicious can be imagined, but one that has been used with success is for students to tag Web sites prior to coming to class and to submit a Web site evaluation form at the start of class. If each student uses his or her initials as the first keyword tag, it is easy for the instructor to match the tagged Web site to the student who submitted it.

A discussion of keywords is important for the smooth functioning of the project since students first need to understand the constraints and freedoms of selecting tag terms mentioned above. For instance, Delicious only accepts one word tags, so users often combine two words into a single tag. It would make searches easier if an individual user could decide as a general policy whether he or she were going to use an underline, a dash, or no separation in a compound tag, i.e. openaccess, open_access, or open-access. Students also initially tend to identify each Web site with a single tag, thus failing to take advantage of the relationships formed through multiple tags. With some strong encouragement, the students do develop the ability to characterize their Web sites using multiple terms.

If the first major advantage of Delicious is in learning to evaluate Web sites and developing a healthy skepticism about electronic content, the second advantage occurs in the lecture. If students are required to tag Web sites in advance relating to a day’s topic, the class can begin by using a computer projection system to take 5-10 minutes for the group to view some of the Web sites. The student who tagged each Web site can explain why he or she found it worthy of note, and the content of the Web site may be used to provide context and examples for the day’s work. Sometimes a single student-tagged Web site may provide an outline of the entire

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lesson plan for the day. Because the students select the Web sites, the students can also introduce information of personal interest to themselves to be included in lecture and discussion. For example, on the topic of pesticides, a student from India tagged a Web site telling of problems resulting from endosulfan application in her own country. A strong interest in cars prompted a student to tag a site about halon fire extinguishers in race cars for the ozone depletion topic. The students, themselves, display a bias when tagging Web sites, since on only one occasion did a student tag a Web site thought to be of poor quality (*16*).

Although a collection of Web sites tagged on delicious is an excellent method for enhancing or embellishing content in a course, it is not an effective substitute for a textbook. Because the content generated by the students is somewhat random, the tagged sites do not constitute a reliable or comprehensive database on a given topic. It might be possible to overcome this limitation if the professor tags Web sites that include fundamental information and skill instruction, but that strategy is less desirable because it would reduce the student ownership of the project,.

IV. Information Presentation and Synthesis: Wikis

Wikis, familiar especially through Wikipedia, have found multiple applications in education. Their power as a group editing tool will be the focus of the current discussion. The use of wikis also teaches the invaluable lesson that the first draft of a product should not be the final draft.

Students inevitably grumble about group work and that all too often, all the students in a group do not pull their own weight. Although various strategies have been employed to attempt to allocate contributions to various students, they often rely on the students in the group to evaluate the contributions of each member. In contrast, wikis feature an edit trail, which allows for two different versions of the project to be compared, highlighting changes made by a particular user and thus assigning contributions unambiguously. The degree of collaboration can be established as well to determine if a product is truly an integrated effort among the group members or if it is multiple individual pieces linked only by cursory connections. Indeed, there is a perceptible difference between projects created from the start to be an amalgamation of ideas and projects involving separate pieces related only through proximity by cutting and pasting content together.

Wikis have been used effectively in a variety of ways, such as group editing of laboratory reports (*19*), group commentary on an article (*20*), and even as a chemistry textbook (*21*). One of the authors of this chapter has used wikis in place of term papers to allow students more freedom to explore topics supplemental to the main outline of the course (*22*). As with teaching and learning any new skill, students must be provided with several opportunities to develop their expertise, so in the latter project, groups of three or four students created wikis on different topics three times during the semester. With each completed assignment, the students demonstrated increased facility with managing wiki content. Spreading assignments throughout the course also resulted in a more evenly distributed workload for students and professor compared to the typical crunch of term papers at the end of the semester. From the faculty perspective, grading well-integrated

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wiki assignments offers special challenges. The evaluation must consider the final version of the wiki as well as the contributions made by each individual to the development of the finished document. The edit history of the wiki, which allows every previously saved version to be viewed and compared to other versions, permits an unequivocal identification of each contribution from each student. Even so, it takes some practice for a professor to develop the ability to evaluate potentially forty or fifty different versions of a wiki to arrive at grades for each individual student.

When each group of students was allowed to select topics for each wiki, the subjects tended to be much more relevant to the course material than the historically more obscure term paper topics, and details of the more deeply researched wikis were used to enhance the breadth of information presented in class. Accountability for fellow students' wikis was also established by allowing students to select exam questions to answer on each wiki, but not allowing the students to answer questions from their own work. The flexibility of the wiki medium shows great promise as a widely adaptable and instructive teaching device

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V. Information in Small Packages: Potential Uses for Twitter

Twitter, the microblogging site that limits messages to 140 characters, is currently the most rapidly growing social networking Web site, and it arouses strong emotions from both proponents and opponents. Twitter is probably best viewed as a rapid-access news ticker, which is best known for providing up-to-the-minute reporting on events like the protests against the Iranian election or the emergency landing of US Airways Flight 1549 in the Hudson River. The 140- character limit on each Tweet creates headlines that can be scanned in seconds and often include links to other Web content for potential further exploration. Thus, it can serve a valuable source of quick information.

The main limitation of Twitter for chemists is that so few chemists are using it. As Mary Virginia Orna (*23*) pointed out, "The ACS Strategic Plan seeks to address a future peopled by youth that has embraced a Web-based culture that communicates mainly by text-messages and Twitter, and by adults who are barely scientifically literate." Despite this insight, it appears that individual chemists are not using Twitter. This conclusion is based on the observation that relatively few individual chemists were tweeting during the fall 2009 and the spring 2010 ACS national meetings, even though a number of companies and American Chemical Society Divisions were using the service.

In order to start using Twitter; simply go to the home page (*24*) and sign up. It is best to also download a program, like Tweetdeck (*25*) that will organizes the Tweets. Tweetdeck organizes the message flow into three basic columns, labeled all friends, mentions, and direct messages. Frequently, discussions on Twitter are organized using a label called a hashtag, indicated by a pound sign (#). This allows a Twitter user to follow some of the questions and comments during presentations at some academic conferences, even if he or she is not physically at the meeting. Often the tag is obvious, for example, #acs_sf was used for the National ACS

Meeting in San Francisco. Tweetdeck allows one to search for a hashtag. Clicking on the small circle with the plus sign in the upper left hand corner of the Tweetdeck screen, and typing a hashtag, like #acs_sf, into the search box will create a new column for tweets having just this tag.

Twitter may also be used for creating a back channel for questions and discussion during classes, but thus far there have been no reports that this is being done for chemistry classes. Dr. Monica Rankin (*26*) reported that she uses Twitter as a back channel in her history courses at the University of Texas at Dallas and Olivia Mitchell has written a free, online book (*27*) that explains how to run a back channel more effectively.

The key to using Twitter for Chemistry is to find other chemists with similar interests to follow. There are several ways to identify individuals to follow on Twitter, such as directories, like Wefollow (*28*), that list people with specific interests, or customized lists of Twitter users, like Listorious (*29*), which list Twitter users who describe chemistry as their special interest. Twitter can be valuable to chemists in several different ways, if enough chemists become involved in using the software. It is hoped that this interest will develop soon.

VI. Information and Image Delivery: Google Jockey

Back channel chat, in which Twitter has found classroom utility, is effectively an electronic method of passing notes. Courageous instructors or speakers will arrange for an additional screen and projector so that the back channel communication is made public to the entire group, potentially identifying issues for clarification or further development. Engaging the back channel dialogue is not for the faint of heart since it requires the instructor to surrender some control of the class, but it consequently carries a great potential for engaging the students in greater participation.

Google Jockeys represent an alternate back channel option that restricts the input to only a few students but vastly expands the range of media contributions. The term was coined by Michael Naimark (*30*), a Professor in the Annenberg School of Communication at the University of Southern California. The original Google Jockey experiment pitted two students against each other to find and project electronic information related to the classroom discussion (*31*). The term has since more commonly referred to students who surf the Web to provide and project visual information related to a class discussion. The interaction between instructor and Google Jockey represents back channel interactions at their most collaborative as well as producing a strong flair of theatre and play.

The power of the Google Jockey is that it allows a student to use his or her own experiences to form connections between discussion and images. Unlike PowerPoint, in which images are pre-selected by the professor for a predetermined line of discussion, the images selected by a student while discussion is in process are far more likely to resonate with the rest of the students in the class, invoking experiences and contexts shared by other students. A student with nimble search skills will also rapidly respond to unexpected tangents and issues so that projected images and dialogue are constantly synchronized. The result is a vastly enriched

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foundation for discussion and presentation that potentially engages distracted students and models effective Internet search strategies (*32*).

For the uninitiated, this mixed format creates a significant challenge since an additional information stream of images or text is added to the professor's comments and the general discussion. During a semester long experiment with a Google Jockey in a first year seminar class (*33*), some of the students initially indicated that the image component of the multiple inputs was a distraction, but at the end of the semester, the class had universally adapted to processing lecture, discussion, and images simultaneously, and they reported that the images greatly enhanced the quality of the class.

Google Jockeying is not as easy as it looks, as has been found by students substituting for the regular Google Jockey. It requires strong Internet search skills plus a simultaneous ability to focus on the current discussion, to anticipate the next topic, and to potentially edit or censor material when an innocuous search in one context might produce inappropriate material from another. It also requires a strong bond of trust between the student and professor that the selection of images and commentary on them will always be done in a respectful manner. With these qualities in place, it is easier for the professor to relinquish partial control of the class in favor of the enhanced engagement of all parties.

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VII. Summary and Conclusions

This chapter is based on two fundamental ideas. The first is that information management is a basic skill which all chemists need to have mastered in order to function effectively in their profession. As noted in the brief introduction, this idea long predates the development of the World Wide Web, although the proliferation of online information sources has certainly exacerbated the problem. Information overload may appear to be an overworked cliché, but it is a phenomenon that is all too real. It seems likely that it will become worse in the years ahead as online information sources multiply, new publication avenues emerge, and countries such as India and China, are increasingly the source of cutting edge chemical research.

The second idea, which may be somewhat more controversial, is that the best way to prepare students to manage information is to teach them these skills as a part of their undergraduate education. Students may know many things about technology, but information management is unlikely to be something that they learn either on their own or in other classes. Much as professors would like to shift the task of teaching these skills to someone else, there does not appear to be anyone willing and able to undertake the job.

Some complain that Web 2.0, the general rubric used to describe the programs discussed here, is just a passing fad or a group of petty designs. The vast majority of college teachers seem to have already rejected this argument. A recent survey (*34*) of college professors by Pearson publishing shows that that 80 percent of professors have at least one account at a major social networking site, and most had an account at more than one site. In addition, a majority of them said that they used social networking sites for teaching. Although results were not specifically reported for chemists, the three groups of faculty surveyed: business

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and economics, humanities and social sciences, and mathematics and science, reported similar results. These results do not focus on the use of sites like those described in this chapter, but it is apparent that many faculty are willing to explore Web 2.0 tools for instruction.

Finally, conversations with some colleagues suggest that "technology fatigue" may also be a factor. Some individuals feel that they have devoted as much time as they can spare to learning new technologies and are unwilling to expend more effort in this direction. There is no doubt that it requires a considerable investment of time to learn how to use new programs and also to evaluate which of several available programs might be most useful. There is no simple answer to this resistance, except that it has become an inherent obligation for teachers in today's world.

Perhaps the best approach for an individual is to choose one of the technologies described in this chapter and use it in his or her classroom. Not every faculty member has to explore every new technique, but it is certainly desirable to be aware of how some of the recent developments might be used in the classroom. The best way to make solid progress is by taking a succession of small forward steps.

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Chapter 8

Preparing for the New Information Paradigm

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The power of the World Wide Web to connect scientists and their work is revolutionizing scholarly communication and education. Web 2.0 tools create new avenues for collaboration, data sharing, and publication. Online journals, open access publications, and eBooks allow educators to augment the chemistry curriculum with current, relevant research. Using these tools, chemical educators can create curricula that are engaging for today's students. If chemistry education is to remain relevant and attract the next generation of scientists, educators must adapt to this new information paradigm.

Introduction - The Changing Environment for Chemical Scholarship

Digital technologies are rapidly integrating into the fabric of academic research. Christine Borgman (*1*) summarizes the situation writing that, "Every stage in the life cycle of a research project now can be facilitated - or complicated - by information technologies." This is equally true for chemistry. Digitization is changing the way that chemists access, store, read, and write articles. Nearly every aspect of the process of scholarship is in flux because of digital technology. One of the key steps in this process has been the proliferation of online scholarly journals. The hyperlinks found in online articles connect documents, information, and people in new ways, changing the way that scholarly research is being done.

Although scientific journals were the first to be affected by digitization, the focus is shifting now to concerns about how data are stored and shared, open access journals, electronic books (eBooks), and, most recently, smartphones.

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

These developments have stimulated new patterns of literature use, the creation of extended scholarly research networks, and a loosely organized movement that is calling for "open chemistry." Collaboration among geographically dispersed scientists is becoming commonplace, part of the e-science revolution. Shared access to databases, remote access to scientific instruments, and high performance computing allow for “dispersed networks of researchers to exchange data and pool computational resources across both time and space” (*2*). Several symposia at National meetings of the American Chemical Society (ACS) have focused on Web 2.0 or Scholarly Communication 2.0 (*3*). All of these changes in chemical research should be reflected in chemical education. Now is the time to reconsider the educational process in order to harness and integrate the next generation of scholarly research tools.

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Online Journals Are Changing the Way Information Is Used.

For more than a decade, chemistry journals have trended toward an online format. The Committee on Computers in Chemical Education (CCCE), of the Division of Chemical Education of the ACS, began exploring online formats in the early nineties. The *CCCE Newsletter* has been online since 1991 (*4*) and in 1993, Tom O’Haver and Don Rosenthal (members of the Committee at that time) organized the first online Conference on Computers in Chemical Education (*5*). ConfChem, as it is called, gathers papers from the international chemical education community about some predefined theme and publishes them online. This is followed by a moderated online discussion of the papers during a specified time frame. The resulting discussion is more structured than an online discussion list, like CHEMED-L, and might best be viewed as a hybrid format between an online chemistry journal and an online conference (*6*).

In his review of the milestones related to online publication of chemistry journals, Garson reports (*7*) that the ACS made supplemental material for the *Journal of the American Chemical Society (JACS)* available online in 1995; however the first ACS journal to be published online was the *Journal of Physical Chemistry* (*J. Phys. Chem.*) This was done in 1996 to celebrate the 100th anniversary of *the Journal*. Prior to their online formats, both *JACS* and *J. Phys. Chem.* were searchable as CD-ROMs (*8*). In the fall of 1996, the *Journal of Chemical Education* also began publishing papers online. By 1997, all 26 ACS journals were available on the World Wide Web. Garson quotes the Editor of the *Journal of the American Chemical Society* as writing, "Electronic publishing and the WWW represent the biggest revolution in publishing and the dissemination of ideas since Johannes Gutenberg invented the modern printing press in 1455."

Garson writes that, "To date electronic-only journals in chemistry have not been well received," but even if ConfChem is not accepted as a true journal, *The Chemical Educator* is an example of an online chemistry journal that began publication in 1996 and is still viable. The editorial (*9*) in the first issue of *The Chemical Educator* suggests that publication on the World Wide Web offers advantages, such as ". . . quick and timely dissemination of articles, immediate availability of supporting material, full-search capabilities for the current and all back issues of the journal, and the ability to include full-color graphics, video clips, and animations. Moreover, through forums, it can provide a communication link between its readers and authors." In 2004, *The Chemical Educator* added a print version in addition to the online publication.

According to Garson, by 2003, 83% of the scientific, technical, and medical journals were available online. The decision by the ACS to focus mainly on online publication (*10*) is not only a suggestion of how fast the scholarly world is changing but also an indication that even greater change is likely. Online publication is important because it encourages new forms of reading and also enables new journal formats.

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Changing Patterns of Behavior by Researchers

Several recent studies have shown that the availability of online journals and reference materials is changing the way in which researchers read the scientific literature. A recent study in *Science* magazine (*11*) reported that scientists are reading more journal articles but are spending less time on each article. This apparently contradictory finding is most likely explained by an English study (*12*) that reports that researchers are more like to "power browse" their way through digital content rather than reading each article thoroughly. The authors of the latter work suggest that researchers are, "developing new forms of online reading that we do not yet fully understand." Although researchers are reading differently, the structure of the peer-reviewed article has not substantially changed, “in particular, semantic information describing content of these publications is sorely lacking” (*13*). Peter Murray-Rust, a chemist at the University of Cambridge, has decried the way “traditional presentations of information in scientific articles, such as graphs and charts, actually obscure or destroy data” (*14*).

Digitization is changing the way that scientists use the library. Every three years since 2000 Ithaka S+R, the strategy and research arm of ITHAKA, has conducted a survey of how faculty use library resources for scholarly projects (*15*). ITHAKA is an organization that supports innovation in higher education. Previous ITHAKA surveys have shown a steadily increasing percentage of researchers start their personal research by using an online search engine or some specific online resource rather than library catalogs or librarians. The 2009 survey indicates that this behavior is reported by about 90% of scientists with somewhat smaller numbers of social scientists and humanities scholars displaying the same behavior. Although this survey did not report results separately for chemists, it is quite likely that their behavior is similar to the scientists in general, particularly now that *Chemical Abstracts* and other major chemistry resources are available online.

As pointed out in a recent report by the Association of Research Libraries (ARL) (*16*) “The networked digital environment has enabled the creation of many new kinds of works that are accessible to end users directly, and many of these resources have become essential tools for scholars conducting research, building scholarly networks, and disseminating their ideas and work.” As the ConfChem experience mentioned earlier demonstrated, online articles can become the basis

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for open discussion and evaluation on the World Wide Web. These new kind of works include journals that are experimenting with new forms of peer review, like *Atmospheric Chemistry and Physics* (*17*) and *Ecology and Society* (*18*) .

Online journals allow new ways to present information, such as the addition of videos, perhaps best exemplified by the *Journal of Visualized Experiments* (JoVE) (*19*), the “first online journal devoted to video publication of biological research.” Videos can be used to clarify the actual procedures used in a process or experiment, to help visualize data correlations, and perhaps most important, to put a human face on the science that is being described. JoVE does include some chemistry videos and the video by Bradley et.al., is an excellent example of the way a chemist might use televised images to help describe his or her work (*20*). The authors use video to demonstrate the use of an unusual scientific apparatus, to summarize experimental results, and to put a human face on the scientific process.

The ACS has begun to include video abstracts for selected articles from the *Journal of the American Chemical Society* (*21*). These videos are summaries of recently published *JACS* articles, created by the authors of the articles. According to a poll that accompanied one video abstract (March 27, 2010), a majority of those who viewed the video responded that they would use it primarily to understand the article better.

In 2007, The Royal Society of Chemistry (RSC) announced Project Prospect (*22*), which adds metadata to selected articles in journals published by the RSC. This metadata allows readers to click on compound names, scientific terms, or experimental data to open drop-down windows on the page that provide further information. This gives readers access to additional articles by the same authors, articles with similar titles, physical and chemical properties for compounds, structures, and definitions. Project Prospect also links to other data sources, like the IUPAC Gold Book, Open Biomedical Ontologies: a hierarchical classification of biomedical terms, and Chemical Markup Language: a chemistry equivalent of the Internet’s HTML. Clicking on an ontology term connects to a definition from the Gene Ontology, Sequence Ontology, Cell Ontology, or ChEBI (Chemical Entities of Biological Interest) listing. A link to the online ontology lists other related RSC papers which have been enhanced and also contain that term. Since the metadata are readable by a computer, this is a step toward the Semantic Web, where the computer searches not just the specific term but also synonyms.

New Forms of Collaboration and Open Chemistry

Digitization is creating new opportunities for collaboration in the classroom and the laboratory. There is a long tradition of scientists informally sharing information and ideas, going back to the "Invisible College" in England in the 17th Century and continuing to the present day (*23*). Using digital technology in the classroom to create a similar collaborative environment for student learning is a more recent development. As early as 1990, Pence (*24*) made a first effort at combining computerized presentations with cooperative learning. By 1996, Theresa Zielinski and co-workers (*25*) had moved beyond a single campus to create a collaborative learning environment at four geographically dispersed colleges to form an intercollegiate learning community. This project continued for several years with participation by faculty and students engaged in the undergraduate physical chemistry course. The materials created by Zielinski, , continue to be available online through the *Journal of Chemical Education* Online under the heading of the *JCE Digital Library, Learning Communities Online* (http://jce.divched.org/JCEDLib/LrnCom/index.html).

Cooperative learning has become commonplace in chemistry classrooms, and there is considerable hope that cooperative, multi-campus projects might become equally prevalent. Students today need this kind of experience, as chemical employers are increasingly placing a premium on the ability of their new hires to cooperate, not just with those at other locations in this country, but around the world.

Several sites on the World Wide Web have been specifically created to facilitate collaboration among scientists. The Scientist Solutions discussion board (*26*) was created in 2004 to provide a space where scientists could discuss scientific problems they encountered. Marcia Allen, the Chairman and founder explains that she was inspired by witnessing the power of eBay to connect people. Although the topics listed are mainly biology and biotechnology there are a number of ongoing discussions about biochemistry and analytical chemistry.

Another Web site that was created to encourage scientific collaboration is InnoCentive (*27*), which was founded in 2001. This site is designed to connect organizations that have specific research goals with a diverse community of experts who are willing to attempt to solve these problems in order to gain financial rewards. The types of assistance invited by InnoCentive include groundbreaking ideas, detailed implementations for an idea that has been developed but not yet proven, the testing of a theory or design, or a partner to provide materials or expertise to help solve a business challenge. The challenges span a broad spectrum of the sciences, but relatively few are related to chemistry at this time. A study of InnoCentive led by researchers from the Harvard Business School (*28*) found that nearly 33 percent of the problems posted on the Web site were solved within the specified time frame and that problem solvers were most effective when they represented a multi-disciplinary team.

Currently, there is a growing movement called Open Science or Open Notebook Science (*29*) which argues for complete public transparency of research results, including a record of the data acquisition and research progress. Open Science hopes to encourage the creation of collaborative communities of researchers, who can contribute to the development of projects. The Blue Obelisk (*30*) is an informal group of "chemists/programmers/informaticians who are driven by wanting to do things better but are frustrated with the closed systems that chemists currently have to work with. They share a belief in the concepts of Open Data, Open Standards, and Open Source (ODOSOS) (but not necessarily Open Access). Most chemists are accustomed to keeping laboratory procedures and in-process data private in order to prevent potential competitors from getting a head start, and because of possible financial rewards, real or imagined, that might result from a patent. A significant change in the values of the profession will be required for the Blue Obelisk-like attitude to become main stream.

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Data Access Is Playing an Increasing Role in the Scientific Literature.

Digitization is not only affecting scientific journal formats and the way that scientists read journal articles; it is also changing the way that scientific data are collected, analyzed, and stored. In many disciplines, including some chemical disciplines, like environmental chemistry and biochemistry, computerized data collection is creating huge databases that can only be accessed effectively by computer. In a recent book (*31*), Tony Hey and co-authors propose a new scientific methodology based on data-intensive discovery. The traditional scientific paradigms are based on theory and experiment. In the mid-20th Century a third approach, large-scale computational simulation, came into being. Hey and his collaborators contend that a fourth paradigm called data-intensive science is now emerging.

Recently, *Nature* magazine devoted an entire issue to the way scientists handle data and highlighted the problem with an editorial titled, "Data's shameful neglect (*32*)." This commentary stated that, "More and more often these days, a research project's success is measured not just by the publications it produces, but also by the data it makes available to the wider community." In many cases a paper version of the database would be so large as to be almost useless. Unfortunately, this often means that the data that accompany an article may not be readily available or may be stored online as "supplemental material." Thus, the data are much less accessible than other parts of the article.

Computerized data analysis is making these databases more valuable. Computers are not only used to collect and store data, but also to analyze it in new ways. Tom M. Mitchell (*33*) points out that ". . . machine learning algorithms have helped to analyze historical data, often revealing trends and patterns too subtle for humans to detect." Powerful data mining techniques are being used to discover subtle patterns that were previously unrecognizable (*34*, *35*). A chemistry-related example of data-mining is the *Cambridge Structural Database (CSD)*, a "computerized archive of bibliographic, chemical and numerical data from X-ray and neutron diffraction studies of small organic and metallo-organic molecule" (*36*). Since 1991, more than 700 papers have been published as a result of applying various methodologies to the CSD. Unfortunately, there are many hurdles to be overcome before universal data access becomes a reality. It is not clear who will curate and store these valuable information resources. Libraries represent logical centers for data storage, but paying for data storage and curation, especially at a time when most libraries are having trouble funding their ongoing activities, is even more problematic than paying for open access.

Attempts to create online data storage sites seem to have met with mixed results. Another article in the special issue of *Nature* (*37*) relates how the University of Rochester (New York, USA) invested US $200,000 to create a digital archive for all types of data and as of the writing of the article the repository was largely empty. One of the administrators responsible for the repository said that, "When the time came, scientists couldn't find their data, or didn't understand how to use the archive, or lamented that they just didn't have any more hours left in the day to spend on this business." According to the article, databases that focus on specific disciplines, like physics, geophysics, and astronomy, seem to have done much better than multidisciplinary sites. Fundamental questions about data standards and data curation still need to be answered.

There are some hopeful signs. Funding agencies, like the Wellcome Trust and the NIH National Library of Medicine, have been very successful at supporting databases in molecular biology, but many scientists are hesitant (or uncooperative) about submitting their data. The U.S. National Cancer Institute has created caBIG® (The **C**ancer **B**iomedical **I**nformatics **G**rid®) to allow researchers, physicians, and patients to share data and knowledge (*38*). In 2008, the pharmaceutical giant, GlaxoSmithKline (*39*), donated a vast library of biological information collected with microarray chips to caBIG®. GlaxoSmithKline apparently hopes that independent researchers will access this data to create new oncology drugs and tests. Both the United States (*40*) and the United Kingdom (*41*) have created linked data sites to act as a central repository for government data. As of this writing, none of these sites has much chemical information that appears useful. However, these repositories represent a commitment to open data by government, and at least demonstrate movement toward the Semantic Web, an extension of the current World Wide Web in which information is stored in formats that are accessible to computers.

How might chemical education be affected by the digitalization of data? Some chemists may be skeptical about the Fourth Paradigm idea, since they do not normally encounter the large databases envisioned by Hey, This would be shortsighted. Chemistry students at all levels need to learn how to use general databases, like ChemSpider, as well as specific databases like those used in biochemistry and molecular structure determination. The editorial in *Nature* mentioned earlier (*28*) highlights the opinion that, "Data management should be woven into every course in science." Specifically, the editorial recommends that all students should have a course in information management that describes how data are acquired, stored, organized, retrieved, and curated. In the long run, this is certainly a desirable goal, but it would be difficult to find room for such a course in the already crowded chemistry curriculum.

For the time being, the most desirable approach is to introduce data management into individual existing undergraduate courses. The obvious locations for such instruction would be biochemistry or environmental chemistry, where data manipulation is already recognized as an important skill. There are a number of software packages that can be used to teach data manipulation across the curriculum. Teaching students how to use spreadsheets, for example, is a common practice in some chemistry courses. A recent search on the keyword "spreadsheet" in the *Journal of Chemical Education* returned over 832 hits. By no means are spreadsheets the only tools to consider. A search of the *Journal of Chemical Education* for the term ‘wiki’ returns 80 hits, and if this search were extended to other ACS journals there are a large number of projects that can serve as templates for undergraduate projects. The work by Zielinski et.al., (*21*) mentioned earlier provides yet another source of suggested projects, and these have the advantage of being designed to coordinate student work from different locations. Finally, Bennett and Pence (*42*) have explored the use of Google Docs as a medium for data sharing.

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Open Access Journals and Chemical Education

Open access journals are becoming a significant component of the information infrastructure in the sciences, providing free, permanent, online access to research articles for any Internet user. John Willinsky (*43*) , in his book defines ten variations of the idea of open access, ranging from journals that select a few articles from each issue as open access (mostly for marketing purposes) to journals that offer immediate and complete access to all articles. Even commercial journals allow authors options for open access; authors can elect to pay a fee in order to make their articles freely available or they may choose to place their publications in an open access repository after a designated period of time.

The open access movement became widely recognized after the Budapest Open Access Initiative of 2001 (*44*). This initiative, sponsored by the Open Access Society, was an international effort to make research from all disciplines freely available on the Internet, and this position has since developed considerable support. The essential characteristic of open access journals is that they are not paid for by subscribers and that the journals are usually funded by a combination of grant support or payments by authors. The cost to publish an article in an open access journal ranges from 500 to several thousand dollars, although most journals will waive the cost for those who do not have support for this expenditure.

A recent article in *Nature* (*45*) raised questions regarding the sustainability of the open access publishing, particularly the model used by the Public Library of Science (PLoS). PLoS, a non-profit publisher of highly regarded open access journals, recently introduced *PLoS One: Publishing Science, Accelerating Research*, offering lower author fees and less intensive peer review. *PLoS One* has been criticized for "bulk publishing" in order to subsidize their high-quality flagship journals *PLoS Biology* and *PLoS Medicine*.

Alternatively, BioMed Central, an open access publisher with more than 190 open access journals, has remained "pleasantly profitable." Late in 2008, Springer, one of the major publishers in Science, Technology, and Mathematics (STM), supported the viability of the open access model by purchasing BioMed Central. The CEO of Springer Science Business Media said, "This acquisition reinforces the fact that we see open access publishing as a sustainable part of STM publishing, and not an ideological crusade (*46*)."

A major motivation for open access publishing is the ability for scientists to freely share and access peer-reviewed research on a global scale; however another factor driving open access publishing is the funding guidelines from government and private institutions. The U.S. Congress passed the National Institutes of Health (NIH) Public Access Policy in 2008. This legislation requires federally funded research publications to be available, at no cost to the taxpayer, on PubMed Central (*47*), and reach the public domain within twelve months after publication. Private foundations in the US and abroad have also been at the forefront ensuring public access to their funded research

Chemists have been less active in exploring new publishing options than other scientific disciplines. According to the Directory of Open Access Journals (*48*), there are more than 5,514 open access journals available online, of which 81 titles are in chemistry or chemical engineering. Of significant interest to chemists

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is BioMed Central, a London-based open access publisher. BioMed Central publishes the *Chemistry Central Journal* (*49*), a peer-reviewed, open-access journal, divided into 55 subject-specific sections.

Some chemistry publishers have responded to open access publishing by offering free public access to articles older than six months or a year (*50*), a process sometimes called “back access.” The Royal Society of Chemistry (RSC) now offers free access to the RSC archives (1841-1996) to scientists in Africa and many of the former Soviet states. Although the ACS has taken a strong position against government mandated open access, it has also instituted its own open access program, called AuthorChoice (*51*), which (according to an ACS Press Release) "allows individual authors or their research funding agencies to sponsor open availability of their articles on the Web at the time of online publication."

An advocate for the use of open access in education, Malcolm Campbell (*52*) reminds educators that “research begins in the literature, not in the laboratory,” and that “the benefit of open-access literature is both obvious and immediate.” Chemical educators can use open access to enhance the undergraduate curriculum by incorporating critical evaluations of research methodologies and results. Students working with real problems from current literature can be encouraged to ask new questions and to design their own experiments. With the increasing demand for access to raw data, educators can foster an environment of innovation.

Open access is not just about scientific research; it is about how scientists should be educated. The editorial in the first issue of *PLoS Biology* (*53*), one of the premier open access journals, stated that one of the main goals of the publication was to, " . . . form a valuable resource for science education." Chemical educators need to understand these new forms of scholarly communication in order to participate fully in the discussion of their discipline and to provide chemical education that is appropriate for the new century.

How May eBooks Change Chemical Education?

The decline of print materials in academic libraries is a factor of changing technology, cost, and declining use. This generation of students, and those that follow, will increasingly acquire their information online, preferably through portable devices. Although eBook development is in the early stages, the recent introduction of improved eBook readers, (the Kindle and iPad), in conjunction with the demands of the e-shoppers, may prove to be the combination that dramatically moves eBooks into the forefront.

Until recently the majority of chemistry eBooks purchases in academic libraries were reference materials. For example, the *CRC Handbook of Chemistry and Physics*, is now available 24/7 as an eBook. In response to the changing needs of users, academic libraries are expanding purchasing plans to include non-reference eBooks from scientific publishers including Wiley InterScience, Springer, and Knovel. These plans are based on subject profiles and follow the traditional book purchasing models of “just in case.” As library budgets continue to decline, a new purchasing model is emerging, the ‘just in time’ or patron-select plan. Libraries are testing the patron-select plans with vendors such

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as MyiLibrary (*54*) that offer eBooks from a variety of scholarly publishers. The third time an eBook is accessed by the users through the MyiLibrary platform, the library is charged for the purchase, providing that "just in time" access.

Textbook publishers are also looking for ways to adapt to the declining print market as more students forgo purchasing textbooks and more educators are linking course content to what is available online. The publishers have begun to promote their e-textbooks by offering students expanded content with hyperlinks, video, and visual representations, all at a lower price. Cost is a critical component because "No matter where consumers buy books, their belief that electronic media should cost less—that something you can't hold simply isn't worth as much money—will exert a powerful force (*55*)."

Although libraries and publishers are making the foray into the eBook market they may still not meet the needs of the users. A criticism lodged by Dan D'Agostino (*56*), a development librarian at a large research library, is that "instead of focusing on books downloadable to e-readers or smart phones, academic libraries have created enormous databases of eBooks that students and faculty members can be read only on computer screens." D'Agostino questions whether academic libraries and the big commercial publishers that serve the academic community will find themselves bypassed, "that their onscreen eBooks are not reaching potential readers" and that they will be "unable to embrace the exploding popularity of e-readers and smart phones as platforms for their content."

D'Agotino's point is well taken as today's tech-savvy middle-school student is tomorrow's college student. It's easy to imagine K-12 schools gravitating toward eBooks as not only a way to engage the younger generations, but also as a cost-cutting measure. Nikam and Rai (*57*) envision such a scenario in their article on e-textbooks where K-12 schools would replace textbooks with eBooks, thereby reducing their book budgets. With the money saved from moving to electronic books, schools could even supply students with eBook readers. In fact this is already happening at a K-12 school in Colorado. The Alexander Dawson School in Lafayette, Colorado, through a partnership with Apple has leased one hundred iPads (*58*). In the fall of 2010, teachers and students will test the iPad, studying the educational benefits, "from making interactive science demonstrations readily available to reducing the cost of textbooks, from integrating Web-based data in history research to improved access to testing materials." For the students, "portable educational devices provide access to lesson materials and eBooks at any time and place thus expanding the opportunities to learn (*59*)."

Even though libraries are purchasing eBooks and educators are beginning to use e-textbooks, there is little research on the impact of eBooks in education or how they are used. Jenifer Demski, writing for *Campus Technology*, recently surveyed three universities that were conducting e-reader pilot studies on their campuses using the Kindle DX or the Sony reader model PRS-505 (*60*). The assigned readings were chosen to avoid color illustrations and complex drawings, since the E Ink electronic paper used in these readers couldn't handle this material. Demski observed that, regardless of the type of reading, college students need to be able to highlight important passages, make marginal notes, and quickly skim through a book for review. Neither of these readers did a good job with these

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tasks, although the Kindle was somewhat better than the Sony reader. In particular, students observed that they missed the ability to quickly flip through pages while reviewing for an examination. Overall, these results suggested that eBook readers are not yet ready for classroom use.

That being said, the library at St. Leo University in Florida recently publicized that eBooks will make up fifty-three percent of the library's collection (*61*). Perhaps this small, private university with a student population of 16,000 is on the leading edge as students will be "able to download eBooks to their computers, smartphones, and iPads." One of the main obstacles to campuses adopting eBooks is the fact that many of these devices fail to comply with the Americans With Disabilities Act of 1990 (*62*).

As previously mentioned, researchers and students are developing new skills in the digital medium, they 'power browse,' moving through the Web horizontally rather than vertically. These new forms of reading are not well understood. The SuperBook Project (*63*) from the University College of London will hopefully provide a better understanding of how college students, faculty, and staff interact with eBooks. Using more than three thousand eBook titles, the SuperBook Project ran for 12 months starting in October 2006 and functioned as an "eBook observatory where behavior could be observed and changes introduced and then evaluated." Through deep-log analysis, this study holds promise for discovering user eBook transactions.

Whether the publishers' venture into the e-textbook market, the librarians "just in time" access to eBooks, or the iPad and Kindle will lead to increased use of eBooks remains to be seen. Perhaps the book needs to be less like a book. Moving beyond static PDFs, the eBook "can integrate video, audio, animation, and even interactive simulation (*64*)." It is these 'extras' that make the eBook a perfect match for chemical education, as "electronic texts will be remixed and mashed up with other digital media (*65*)." Interactive and visual representations of chemistry laboratory experiments with hyperlinks to video will become the norm. An example is *CHEMystery: An Interactive Guide to Chemistry* (*66*), designed for high school students. This virtual chemistry textbook, with audio and video components, expands student learning through interactive links to other Web resources.

In addition, eBooks can easily accommodate virtual collaborative authorship through a wiki-like construct (*67*). Wikipedia, the most famous example of the wiki construct, is currently developing Wikibooks, "a free library of educational textbooks that anyone can edit (*68*)." Ravid, Kalman and Rafaeli (*69*) describe in their paper a wikitextbook developed through the co-authorship of undergraduates and graduate students across several universities. These authors suggest that wikitextbooks can empower both students and teachers, and that the use of this so called "disruptive technology" will improve both the student and the curriculum.

Rudy Baum (*70*), Editor-in-chief for *Chemical & Engineering News* (*C&E News*) asked, "Is it possible that reading words is a transient phase in our evolution as story tellers and information exchangers?" and "will people choose to receive the information they need by listening and/or watching rather than by reading?" eBooks and wikitextbooks provide the means to tell the chemical story though hyperlinks, videos, and visual representations. This convergence of text and media may revolutionize chemistry education.

The Ways To Access Information Continue to Change

With incredible rapidity, the cell phone has become an integral part of world culture. Ever since it first appeared in 1973, the mobile phone has steadily decreased in size and increased in ubiquity. It is no longer unusual to see people, especially young people, walking (or driving) with a phone pressed to their ear, deeply involved in some conversation. If not conversing by voice, the individual is equally likely to be sending a text message. Katz and Aakhus (*71*) describe this new environment as "perpetual contact."

The smartphone (such as the iPhone, Droid, or Blackberry), is the Swiss Army knife of modern communications. It combines a phone with a GPS, camera, a compass, and an accelerometer. This enables the device to not only establish exactly where it is located, but also to determine which direction it is pointing and how much it is moving. The power of these features is expanded by the over 150,000 inexpensive applications (apps) that are available for the iPhone, not to mention the ever increasingly number of apps for the Android cell phone operating system. As early as 2004, Bryan Alexander (*72*) predicted that the combination of wireless technology and mobile computing would transform the educational world. He argued that this device would make the information and communications power of the Internet available without regard to time or location. Alexander's predictions are coming true; the smartphone is becoming a significant tool for personal collaboration and interaction.

There are a number of useful chemistry apps available for the iPhone, as described by Antony Williams (*73*). Perhaps the most generally useful of the apps mentioned is one called ChemMobi, which is being made available for free by Symyx Technologies and the Royal Society of Chemistry. This application gives the user access to the formulas, structures, and MSDS sheets for 30 million compounds. In addition, the ACS has recently announced an iPhone app called *ACS Mobile*, which provides a live stream of articles from the Society's research journals as well as a "latest news" feed from *C&E News* (*74*). This application also offers search by author, keyword, title, and abstract, over the entire database of ACS Web editions. Obviously, the use of smartphone apps for chemical education is a potentially valuable topic that is just beginning to be explored.

Perhaps the most surprising use of the smartphones is the large number of people who are viewing movies and TV shows on the small screen. In his blog, Joshua Kim suggests that the willingness to view content despite the small size of the cell phone screen indicates that educational content will soon be moving in the same direction (*75*). He predicts that, "Curricular content will be consumed in shorter chunks, across more diffuse times, and in multiple places." He explains this by saying that content is becoming much more available, so lack of time is becoming the limiting factor. People, both traditional students and adult learners, will want to view small chunks of material when they have time and access. He argues that colleges may begin to have the same problems that currently afflict

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the big three TV networks, competing for attention where once they had little competition.

Conclusion

Ever since the publication of Thomas Kuhn's book, *The Structure of Scientific Revolutions* (*76*) terms like new paradigm and paradigm shift have become so common as to be clichés. Any use of these terms, as in the title of this chapter, must be carefully examined to determine whether they are appropriate. In his book, Kuhn wrote that a paradigm was the philosophic framework that defines a scientific discipline. Normally, a new discipline paradigm will replace the previous practices, although this process may be rather slow. Thus, the oxygen theory of combustion, an example that Kuhn uses, did not supplement but rather replaced the preceding phlogiston theory. The question then breaks down to whether or not the information changes described above are changing the way that scientists are using information to answer the key questions in their disciplines.

The evidence presented above indicates that there are, indeed, major changes occurring in the way scientists collect, access, and store information. This is not just requiring new ways to work, but new ways to access and report information. Surely, this meets the criterion for a true paradigm shift. The most important question is how scientists in general, and chemical educators specifically, are responding to this change. The authors of this chapter would argue that these developments must be accompanied by significant changes in the way chemistry is taught.

Working in this new information environment must become a more significant component of undergraduate education. Power browsing may be an effective solution to the problem of handling too much information, but a good scientist must also be able to burrow deeply into a single source when that is appropriate. Telling students they should be able to do this is unlikely to be very successful. Students need to experience situations where both types of reading are necessary, so they can see the advantages of both approaches. These types of experiences must be integrated into their curricula.

The essential change in the nature of the new information environment is not just that computers have become ubiquitous, but that this ubiquity has created an unprecedented level of interconnectedness. The World Wide Web is no longer mainly about connecting static Web pages of information; it now connects people and creates new opportunities for collaboration. Social interaction, sharing data and ideas across the Web, is the new paradigm that must also become an integral part of the educational process.

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Chapter 9

Integrated Learning Environments: From eBooks to e^{2}Books: From e-Learning 3.0 to e-Knowledge and Beyond

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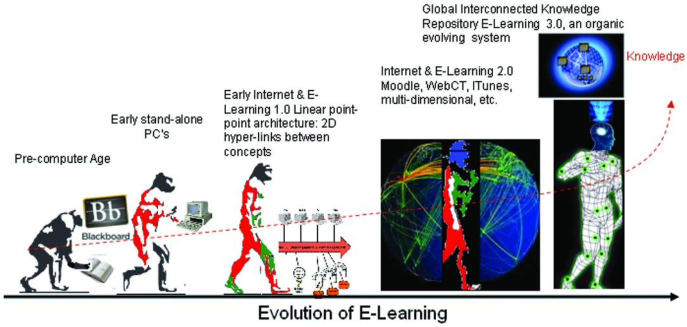
Global Interconnected Knowledge Repository E-Learning 3.0, an organic evolving system
Knowledge
Internet & E-Learning 2.0 Moodle, WebCT, ITunes, multi-dimensional, etc.
Early Internet & E-Learning 1.0 Linear point-point architecture: 2D hyper-links between concepts
Early stand-alone PC's
Pre-computer Age
Bb
Blackboard
Evolution of E-Learning

Original Artwork. Evolution of Man portion from http://anthropology.net/.

The ability to access information has gone through a dramatic revolution in the past few decades. Online e-learning has also undergone a revolution wherein virtually all universities have provided courses that can be taken asynchronously, anywhere and at anytime. Tools and technologies have rapidly evolved to transform the conventional sequential unidirectional methods into collaborative omni directional learning environments. Piaget's theory of cognitive development stated that "the learner must be active; he is not a vessel to be filled with facts…Learning involves the participation of the learner" (Piaget, J. The Child's Conception of the World; Routledge and Kegan Paul: London, 1928).

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

eBooks and new collaborative learning software allows us to create materials and an environment that allow students to explore and independently navigate tendrils of interconnecting concepts that will empower and enhance their construction of a more cohesive understanding of interconnected facets of a discipline. This chapter traces the evolution of e-learning and eBook technologies and explores the current efforts to create more effective e-materials integrated into curricula. Two studies are presented that evaluate the efficacy of e-learning technologies. The first study describes the Kindle Project whose goal is to evaluate the integration of eBooks into university curricula. A second, multiyear study is also presented that evaluates the potential educational benefits of creating an integrated learning environment that allows students the ability to navigate and connect concepts between courses that span a discipline. We are at a critical juncture in human civilization where we have the ability to create a truly global integrated knowledge repository, where material and concepts can be woven together to present courses/materials that incorporate the breath and depth of our scientific knowledge. The challenge is to make these enabling technologies available to all and to create a community that fosters cooperation.

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Learning Objectives

By the end of this chapter the reader will be able to:

a. Describe learning technologies that contributed to current e-Learning paradigms
b. Explain the learning philosophies underlying interactive e-Learning
c. Describe the current state e-Learning technologies and formats
d. Discuss the issues involved in adopting eBook technologies
e. Identify Interactive learning concepts applied to e-Learning
f. Identify new techniques available to create Integrated Learning Environments

1.0. Introduction

The human brain integrates a wide range of data distributed linearly in time into a multidimensional time-independent representation that creates a framework for our perceptions of reality. The goal of an e-Learning knowledge repository is to create a synthesis of information wherein content and context are woven into a tapestry of knowledge. We are at an important juncture in human civilization where we have the ability to create a global knowledge base to provide equal access to information. Until the latter part of the twentieth century, educational institutions acted as guides to provide structure and meaning to disparate facts.

The ecological Gaia hypothesis states that “the earth’s biosphere is an integrated complex interacting system sharing information” (*1*). The potential to provide a technological Gaia where information is linked and integrated into a global knowledge repository is on the horizon. The challenge is to create the tools and mechanisms to support an organic evolving integrated knowledge repository with the ability to link concepts. We have begun that journey with the Web and global search engines. Repositories, such as the National Science Digital Library (NSDL), ChemDB (chemical repository), CIMAP (botanical repository), PubMed (Medical Repository), and NSFCSCR (computer science course repository) have the potential to provide universal access to information. By integrating the conceptual threads that link ideas, we create a technological version of the Arachene Greek tapestry of knowledge, with the potential to accelerate knowledge sharing and create a true tapestry of knowledge.

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2.0. e-Learning and Web Background-History

The precursor to e-Learning was the correspondence courses offered by educational institutions in the late nineteenth century. One of the first of these was offered by Illinois Wesleyan University in 1874 in which course materials and exams were mailed to students (*2*). Most schools depended on honor codes to ensure honest completion of materials. Professional degrees often required verified proctors administering terminal exams. For the next one hundred years a number of variations appeared which incorporated the latest technology available at that time. For example, audio and visual media, such as records and videotapes, supplemented the written materials. In 1953, with the advent of television, the University of Huston offered televised courses. A few universities provided telephone-based feedback from students, but these video presentations were primarily a unidirectional learning environment. In 1960, one of the first distance learning environments to provide real-time student feedback, was the PLATO (Programmed Logic for Automated Teaching Operations) learning system which ran off a 1955 era ILLIAC I (*Illinois Automatic Computer*), similar to the ORDVAC 1 (figure 1). This vacuum tube based computer at the university of Illinois, provided students with the ability to communicate with instructors through dedicated remote terminals. It had 5K of RAM, 64K of Drum/disk memory and weighed 5 tons. The ILLIAC I system had to be shut down every night to test the vacuum tubes. This early e-learning system was funded by ARPA (Advanced Research Projects) which evolved into ARPANET in 1969, the parent of the current Internet.

During the late nineteen sixties and early nineteen seventies a number of efforts provided the building blocks for current e-learning systems. An example of those early systems was COURSEWRITER by IBM, an interactive computer aided (CAI) instruction system that provided real-time feedback for a handful of courses at Stanford University in 1965. During this period parallel efforts were taking place in Canada, France and England. Advanced versions of PLATO III and IV were also tested at Stanford. A number of innovative user interfaces and tools, that would make PC’s more accessible and user friendly, were developed at the Learning Research Group (LRG) at Xerox PARC. This included Graphical User Interfaces (GUI's), folders and menus and Smalltalk, a learning programming language. The Xerox PARC innovations were incorporated in the LISA computer and later in the first APPLE computers.

Computer Conferencing systems were developed in the early seventies and were originally designed to bring together geographically dispersed experts during crises. One of the first of these systems was created by Murray Turoff and Roxanne Hiltz. Called the Computerized Conferencing and Communications Center (CCCC) and the (Electronic Information and Exchange System) EIES (*3*), it was used to create virtual classrooms at the New Jersey Institute of Technology. The later EIES system was used for early e-Learning courses. In the mid seventies Cyclops, an Open University (OU) project, was started in England. It incorporated Whiteboard systems which allowed users to draw and share notes across distances. A few years later, the OU piloted a distance learning system called OPTEL that utilized dial up modems to connect to the remote system.

BITNET, developed in 1980-1991, was created to connect a number of Canadian and U.S. universities. It provided email and online work groups to allow for collaboration. A number of dial up bulletin board systems also provided general connectivity until the advent of the Web/Internet in the nineties.

Beginning in the early nineteen eighties, personal computers such as IBM PC, Apple II, Compaq, Atari, and TRS-80 from Radio Shack, were primarily connected by a series of low baud rate modems, before the higher bandwidth World Wide Web (WWW) became more widely available in the mid to late nineteen nineties. Sir wrote a paper in 1989 (*4*) describing a hypertext linked system, accessible by browsers, modeled after the Dynatext SGML reader, which created the underpinnings of the technology that is used today in eBooks. The first Web server built by Tim Berners-Lee became available in August of 1991 and marked the starting point of the Internet. The Uniform Resource Locator (URL), the Uniform Resource Identifier (URI), the publishing language Hypertext Markup Language (HTML) and the Hypertext Transfer Protocol (HTTP) provided the tools to allow systems to easily connect to the Internet. The WWW.W3.org consortium established and continues to provide standards for protocols and connectivity.

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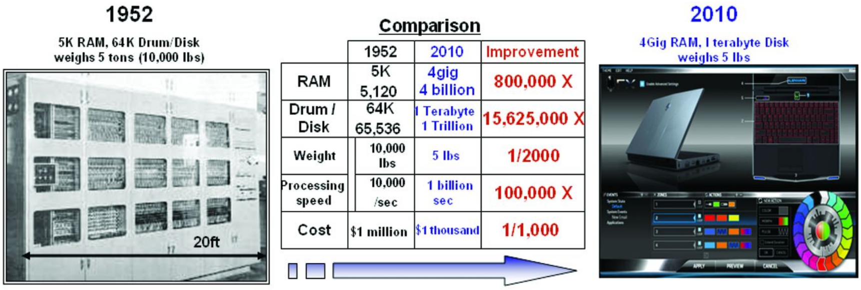

Comparison

	1952	2010	Improvement
RAM	5K 5,120	4gig 4 billion	800,000 X
Drum / Disk	64K 65,536	1 Terabyte 1 Trillion	15,625,000 X
Weight	10,000 lbs	5 lbs	1/2000
Processing speed	10,000 /sec	1 billion sec	100,000 X
Cost	$1 million	$1 thousand	1/1,000

Figure 1. ORDVAC 1, 2800 vacuum tubes vs. avg. quad core PC 4-8 Gig. RAM. Composite of illustrations from: "U.S. Army Photo", from K. Kempf, "Historical Monograph: Electronic Computers within the Ordnance Corps" and www.dell.com.

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2.1. Learning Paradigms

Current e-Learning paradigms embody a more symbiotic relationship between participants. Initial incarnations involved unidirectional, teacher centric dissemination of information albeit with physically separated participants. "*We believe that the most valuable activity in a classroom of any kind is the opportunity for students to work and interact together and to build and become part of a community of*" (*5*). Research indicates that creating omni-directional learning environments with access to external resources allows students to explore and tailor the environment to mach their individual learning styles (*6*).

2.2. Instructional Philosophies

There are three approaches to learning that have evolved during the last century; Learning as response strengthening, learning as knowledge acquisition and learning as knowledge construction (*7*). The first approach has the learner passively receiving reward and punishments, such as drill and practice, simple response and feedback. The second has students placing new information in long term memory. The learner still passively acquires information from the teacher who presents information in textbooks and lectures. Knowledge is a commodity transmitted from the teacher to the learner. The third approach, learning as knowledge construction, is based on the concept that learners actively construct a knowledge representation in working memory. This paradigm, with multidirectional flow of information, represents the framework for current e-learning systems.

In the early nineteen hundreds, Piaget's theory of cognitive development in children (*8*) postulated a sequence of four qualitatively distinct stages of intellectual development; Sensor-motor, Preoperational, Concrete operations and Formal operations. He believed that "the learner must be active; He is not a vessel to be filled with facts…Learning involves the participation of the learner". Creating an environment designed to allow students to explore and independently navigate tendrils of interconnecting concepts will empower and enhance their construction of more cohesive understanding of interconnected facets of a discipline. Later, Vygotsky's (*9*) *Zone of Proximal Development (ZPD)* stated that the potential for cognitive development depends on social development. Skills that can be developed in collaboration with peers exceed those which can be attained alone. This supports the hypothesis that collaborative e-learning can be used to increase social interaction in learning environments and can potentially increase knowledge acquisition. In the nineteen nineties, theories based on human learning in realistic settings (*10*) emerged, in which the learner is the sense-maker and the teacher is the cognitive guide who provides guidance and modeling on authentic academic tasks. The instructional designer's role is to create environments in which the learner interacts meaningfully and fosters the learner's process of organizing and integrating information. The goal is to foster problem solving and conceptual development. Objectivist conceptions of learning assume that knowledge is individually constructed and socially co-constructed

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by learners based on interpretations and experiences in the world. The goal is to *"engage learners in meaning making (knowledge construction)"* (*11*).

3.0. e-Learning in Education Today

As of 2007, ninety seven percent of all community colleges and eighty nine percent of four year public colleges offered distance learning courses (*12*). In 2006–07, there were approximately 11,200 college-level programs that were designed to be completed through distance education. There were also an estimated 12.2 million enrollments (or registrations) in college-level credit-granting distance education courses. It is estimated that virtually all universities will incorporate e-learning into their curriculums eventually. Distance education is defined as, a formal education process in which the students and instructor are not in the same place. Thus, instruction may be synchronous or asynchronous, and it may involve communication through the use of video, audio, computer technologies or by correspondence.

With the almost universal introduction of distance learning courses into university curriculums, new approaches need to be taken to advance conceptual learning strategies that utilize all the resources and speed of this new medium. Some of these are summarized in Table 1.

The next evolution to Integrated Knowledge Repositories is poised to take online instruction to the next level and will be facilitated by efforts of publishers who have begun providing configurable eBooks.

In the last five years eBooks publishing has grown at a rate consistent with Moore's Law, doubling every 18 months (*13*), and is projected to continue at this rate. Generation X, born after the Vietnam War, has never known a world without computers and videogames. Students are not only predisposed to this natural evolution but expect Web-based aids and materials in their education. In the mid nineties the Internet became ubiquitous with instant communication becoming the norm. Online classes have similarly expanded

With the introduction of a number of e-Readers and the evolution of Web-based news access, online courses, online shopping and Web enabled phones, the movement toward eBooks and eventually e-Knowledge, integrating concepts within and across disciplines, is in the process of becoming a reality.

4.0. Electronic-Books (eBook)

An eBook is defined as the electronic counterpart of a printed book, which can be viewed on a computer or a portable device such as a laptop, PDA or eBook reader. (*16*). This basic definition implies a relatively static representation of the original document. However, as e-Learning 3.0 evolves toward e-Knowledge, a more dynamic description is needed. The most popular eBook readers circa 2010are; Kindle, Nook, Sony and IPAD which are illustrated in figure 2.

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Table 1. e-Learning Terminology

Distance Learning / E-Learning /Emergent Learning (a brief summary of terms and concepts)	
Computer Mediated Communication (CMC)	Uses computers and telecommunications networks to compose, store, deliver and process communication *(15)*
E-Learning 1.0	Unidirectional educational modules transmitted to learners
Asynchronous Learning Networks	A form of e-learning that emphasizes the use of the internet to support class discussions and activities. *(14, 15)*
E-Learning 2.0	Follows the philosophy that learners construct meaning as a collaborative effort. Examples: social learning and Omni directional information exchange.
Computer Supported Collaborative Learning (CSCL)	Collaborative group learning using enhanced web 2.0 tools to create an environment for learners to collaborate on learning tasks. Examples:WebCT and Moodle
E-Learning 3.0	Organic, evolving learning environments that form and extract knowledge from ever growing knowledge repositories and incorporate peta-apps that mine data from the web and incorporate this into the knowledge base
Virtual Learning Environments (VLE's) • Shareable Content Object Reference Model (SCORM) for sharing information in VLE's	One or more software technologies to facilitate E-Learning in Education. This has been facilitated by the Open Courseware (OCW) movements. This also includes immersive virtual 3D worlds such as Second Life integrated with Moodle (Snoodle) and Active Worlds
Emergent Learning	It is the process by which simple entities or systems self-organize to form more complex systems. It implies adaptation to the environment, timeliness and flexibility

e²Books would be defined as a dynamic representation of an eBook whereby concepts can be linked to any data source, both internally and externally. The presentation of information could be modified to reflect the needs of the course or audience without changing either copyrighted content or the meaning of that content as intended by the author. Multimedia content is often integrated. Additionally, standard semantic (*17*), terminology, shared by a discipline is often used to link these *e²Books* to knowledge repositories.

Another important aspect of creating knowledge repositories is to digitize existing libraries while observing all copyright laws. As of early 2010, Google Books is in the process of digitizing seven million books, and has reached an agreement with publishers to provide compensation for authors and publishers. As part of the Google Print Library Project it has developed agreements with numerous libraries such as the NY Public library, Harvard, Stanford and Oxford, to digitize books in their collections that are not usually available outside their universities. These books, with certain restrictions, are available at http://books.google.com/?PHPSESSID=f8fdae66572b24ab8fc567c25fbccdc.

Digital Rights Management (DRM) is defined as the process of protecting copyright information on digital content and limiting copying, printing and sharing of eBooks. Adobe PDF documents encrypt the data when they are created. Microsoft reader uses the .lit extension and embeds a digital ID tag to identify the owner of the eBook. There are a number of national and international treaties and laws designed to protect copyright information. The U.S. Digital Millennium Copyright Act (DMCA) passed on May 14, 1998, criminalizes the production and dissemination of technology that allows users to circumvent technical copy-restriction. In 1996 the international WIPO Copyright Treaty (WCT) requires nations to enact laws against DRM circumvention.

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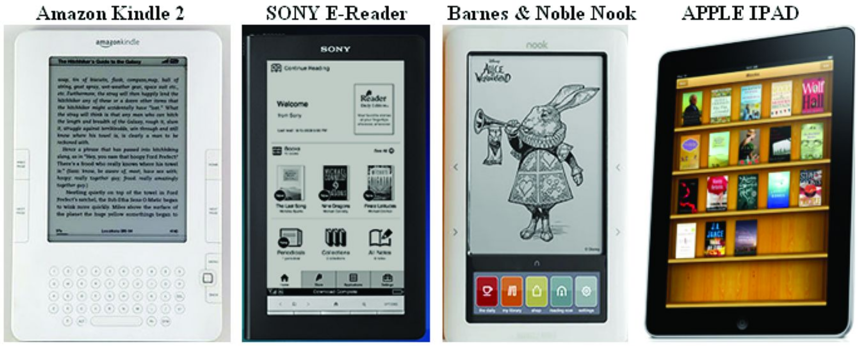
4.1. eBook Formats

A major problem with eBooks is the many competing formats, including Adobe PDF, Kindle Reader AZW / Mobipocket and EPUB open eBook format. Table 2 lists a few of the eBook formats and contains a link to a more complete list of the approximately fifty formats available.

4.2. eBook Technology

Electronic Paper is the generic term for an extremely thin flexible display that can be rolled up. This type of display is expected to become available widely by 2015. The first *electronic paper* was developed at Xerox's Palo Alto Research Center (www.parc.com) in the 1970s. It used a thin sheet of Xerox Gyricon plastic, containing millions of charged beads with black and white hemispheres. This original technology did not work well and was never commercialized.



Amazon Kindle 2 SONY E-Reader Barnes & Noble Nook APPLE IPAD

Figure 2. ***A Sample of eBook Readers (circa 2010).*** *eBook readers from: www.amazon.com, www.sony.com, www.barnesandnoble.com and www.apple.com.*

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Table 2. eBook publishing formats

Popular E-Book Formats (There are approximate fifty formats which can be found at) http://wiki.mobileread.com/wiki/E-book_formats	
Format	**Specifications**
AZW	Amazon's proprietary DRM-restricted format.
Mobipocket (MOBI, PRC) Kindle (2007) & IPhone App	- Kindle 1 (2007) (E-Ink Technology) - 4 gray scales - Capacity 200 books - Kindle II (2009) (E-Ink Technology) - 16 gray scales - Capacity 1500 books E Ink Corp makes electronic paper display (EPD) subsystems for handheld devices using E Ink Vizplex Imaging Film contain microcapsules filled with fluid and many charged black and white particles composed of ink pigments that do not need additional power after initial image is displayed
ePUB.	An open format defined by the Open eBook Forum of the International Digital Publishing Forum
ISO 8859-1	(Latin 1) character set content
OPF	An XML-based e-book format created by E-Book Systems.
PDF	Portable Document Format created by Adobe for their Acrobat products. It is the standard for document interchange. Software support exists for almost every computer platform and handheld device.
TPZ	topaz format books

In 1997, EPD technology was derived from the work of Dr. Joseph Jacobson of MIT Media Labs that improved the electronic paper which had been developed at Xerox PARC by using larger beads and more power. E Ink Corporation was founded to refine the MIT technology.

The Organic Light Emitting Device/ Diode (OLED) is a display technology that offers bright, colorful images with a wide viewing angle, low power, high contrast ratio and fast response time for sports and action movies. OLEDs also have great potential for general use as thin, flat lighting panels that can be mounting on the wall (*18*).

Passive matrix OLEDs began to appear in small-screen devices such as cell phones and MP3 players in the late nineteen nineties and active matrix OLEDs followed beginning in 2003. In 2007, Sony introduced the first active matrix OLED TV and, along with Toshiba and Samsung, announced plans for larger OLED TVs. In 2009, the OQO company introduced the first active matrix OLED screen in a handheld Windows computer.

4.3. eBook Case Studies (Kindle)

A number of studies are in progress to evaluate the efficacy of using this first generation of e-readers/e-text books. The Kindle Project, a multicenter study being conducted at a number of universities, including Arizona State, Princeton, Reed College, Darden School of Business and Case Western Reserve, are integrating

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Kindle and eBooks into their curriculum. The scope and size of the research population vary among the colleges.

Recently, textbook publishers Cengage Learning, Pearson, and Wiley, together representing more than 60 percent of the U.S. higher education textbook market, announced that they will begin offering textbooks through the Kindle Store in the summer of 2010. Even though a number of bookstores are offering a large portion of their books in e-format, the numbers are still relatively modest overall. Besides the MobiPocket format, Kindle also offers books in PDF (*19*).

Case Western Reserve has given Kindles to about 40 students in three courses and is comparing their reading performance, note taking skills, and retention of information with a control group in the same courses who use conventional books. Arizona State's first experiment will be significantly larger, focused on the approximately 1,000 students in its honors college.

Most of the studies are in the early stages, but some initial results reported by Princeton University in the Princetonian indicate that, "In spite of the cost savings, some students and professors said they found the technology limiting" (*20*). The small initial study experimented with the use of the Kindle DX in three courses during the Spring 2010 semester. Another goal was to reduce printing costs on campus. Students in the course WWS 325: Civil Society and Public Policy, who were given Kindles, printed an average of 762 pages, compared to the roughly 1,373 pages printed in prior years. This reflects a 55 percent difference in paper use. Students and professors also reported that, "Despite the Kindle's environmental friendliness, users said they often found its design ill-suited for class readings. Students and faculty participating in the program said it was difficult to highlight and annotate PDF files and to use the folder structure intended to organize documents, according to University surveys. The inability to quickly navigate between documents and view two or more documents at the same time also frustrated users."

4.4. General Purpose Tablets Utilized as e-Readers

The initial response to e-readers may simply reflect the limitations of first generation technology. The devices, such as Kindle, had platforms that locked the users into a limited set of capabilities. This will probably be remedied by a new class of devices with enhanced capabilities, such as the IPAD, and tablets from DELL, ACER, and HP, which will incorporate more general purpose Web access.

In addition, publishers are offering a new suite of tools to allow universities, before disseminating eBooks to students, to customize the presentation by adding video and links to other materials. McMillan publishing now offers *DynamicBooks*, with the description, *"Professors will be able to reorganize or delete chapters; upload course syllabuses, notes, videos, pictures and graphs; and perhaps most notably, rewrite or delete individual paragraphs, equations or illustrations."* This courseware eBook flexibility and an open technology platform with Web access should provide the tools to migrate to an e^{2}Book paradigm.

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5.0. Integrated Learning Environments (Case Study)

An Integrated Learning Environment (ILE) enables learners to explore and independently navigate the tendrils of interconnecting concepts linking a discipline, to facilitate a more cohesive understanding of those concepts. The aim of an ILE is to achieve a quantifiable improvement in learning outcomes by integrating course materials in a field of study. Another facet of an ILE is a knowledge repository that incorporates an adaptable architecture that allows for evolution and growth. An Integrated Learning Environment must be framed around a unifying model and philosophy that supports omni-directional learning. A Constructivist Learning Environment (CLE) (*5*, *21*) is an instructional design theory that is based on the concept that learners actively construct a knowledge representation in working memory. By incorporating these features, an adaptive ILE can be constructed to enhance learning outcomes and provide a cohesive view of a discipline.

The following section describes a multiyear research study that evaluated an Integrated Learning Environment (ILE), using qualitative and quantitative instruments. The hope is that an ILE will be incorporated into a future e-Learning environment that creates e-Knowledge architecture with associated linked e^{2}Books. This ILE is defined as an "*evolutionary environment that links dynamic electronic books, knowledge repositories and provides organic growth to ensure the relevancy of the learning environment.*" Relevancy refers to the *"continuous integration of new content, ideas and feedback to reflect evolving ideas and technologies."* The results of this research illustrated the potential for incorporating an ILE into a leaning environment and enhancing learning outcomes. Students utilizing the integrated knowledge repository achieved a twenty five point increase in test scores on a comprehensive exam versus students completing a conventional course of instruction without the benefit of an ILE (*6*).

5.1. Architecture of the Knowledge Repository for the ILE

A knowledge repository design artifact, the Constructivist Unifying Baccalaureate Epistemology (CUBE) (*6*), incorporating conceptual mapping features and a semantic ontology structure was developed and evaluated in this multi year study. The aim was to determine if quantifiable improvements in learning outcomes could be achieve by integrating course materials within a field of study. The CUBE knowledge repository was modeled as an organic structure with the ability to evolve over time by incorporating a ranking/voting feature which enabled learners and instructors to add further content to the knowledge base and collectively evaluate the relative weights of conceptual threads.

The CUBE artifact was evaluated using a case analysis rubric (table 3). Case analysis problems are often complex, interdisciplinary problems. These problems engage the learners in understanding and resolving issues. They require learners to critically analyze situations, identify issues and assumptions and engage in reflective thinking. The levels of learning and thinking required by this process are at a much deeper level than traditional lecture pedagogy.

An intuitive interface with learner feedback was created to ensure that learners and instructors embraced the Integrated Learning Environment and to facilitate their navigation through the knowledge repository. Learner feedback was provided by semi-structured interviews and a focus group. Students majoring in Computer Technology and Electrical and Computer Engineering Technology at the New Jersey Institute of Technology (NJIT) participated in the evaluation and feedback process. This two-year study involved 90 students in four courses with control and treatment groups utilizing qualitative and quantitative components.

Individual courses are represented as planes on a cube, figure 3, and each box represents an individual topic, or learning object that is linked by a series of pointers to other topics.

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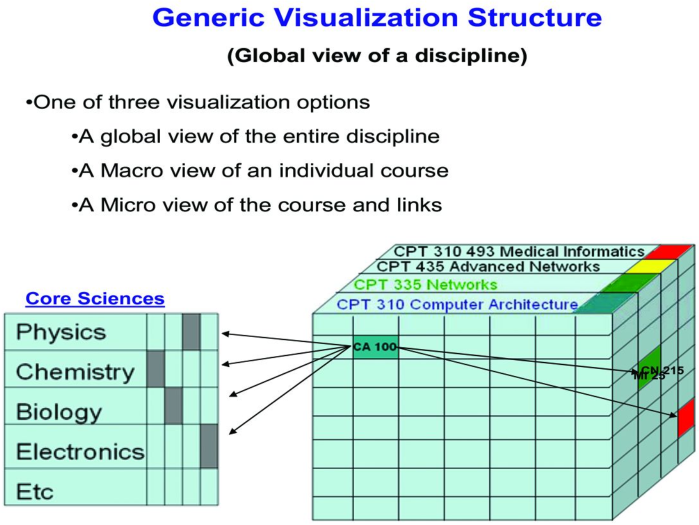
Table 3. Case Analysis Rubrics

Case Analysis Rubrics	
Quality of Information Sources	Sources were internationally recognized; questionable or unknown
Cited (QISC)	
Constraint Analysis (CA):	Constraints are all identified; mostly identified or few constraints known
Feasibility (F):	Feasible to implement; unclear if feasible or impossible to implement
Relevance of Implications (RI):	Implications clear and feasible; implications unclear or few implications identified



Generic Visualization Structure
(Global view of a discipline)
•One of three visualization options
•A global view of the entire discipline
•A Macro view of an individual course
•A Micro view of the course and links
Core Sciences
Physics
Chemistry
Biology
Electronics
Etc
CPT 310 493 Medical Informatics
CPT 435 Advanced Networks
CPT 335 Networks
CPT 310 Computer Architecture
CA 100
CN 215
MI 25

Figure 3. Generic visualization structure linking concepts. (see color insert)

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5.2. Semantic Framework

The Semantic Web (*17*) provides a common framework that allows data to be shared and reused across applications, enterprise, and community boundaries. The semantic theory provides an account of meaning in which the logical connection of terms establishes interoperability between systems and heterogeneous data sets. The ability to generate complex associations between objects provides the potential to link and grow concepts beyond simple document retrieval.

Students evaluated the semantic data collected and ranked their top five choices (Table 4). Following Bloom's Revised Taxonomy (*22*) students rank the quality of the links and content in terms of three categories: Factual Knowledge, Conceptual Knowledge and Procedural knowledge. They are clustered using concept clustering for each generated class using a COBWEB data structure where each node represents the top five highest ranked composite score.

5.3. Quantitative Analysis of the ILE

The goal of this assessment phase was to validate the hypothesis that "Students utilizing the ILE would develop a more complex understanding of the interconnected nature of the materials linking a discipline than those who take conventional single topic courses."

In order to test this hypothesis it was necessary to collect quantifiable data. An exam that covered material spanning multiple courses and evaluated whether students attained higher scores, was created from a composite of exams provided by instructors in the courses. The exam was administered to control and treatment groups. The results supported the hypothesis. The means of the treatment group test scores were 79.41 versus scores of 53.68 for the control group; A difference of 25.73 points higher for the treatment group. This indicates a clear improvement in scores, utilizing the knowledge repository (Table 5 and Figure 4).

Table 4. Ranking Semantic terms used to populate a concept map

Ranking / Voting Links (example)						
Course	**Links**	Ranking 1-5	Factual Knowledge	Conceptual Knowledge	Procedural Knowledge	Mean
CPT 435 Lecture 7	• http://en.wikipedia.org/wiki/Cyclic_redundancy_check	1	67	74	73	71.33
	• http://en.wikipedia.org/wiki/Packet_(information technology	2	63	65	65	64.33
	• http://en.wikipedia.org/wiki/Parity_bit	3	69	53	64	62.0
	• http://computer.howstuffworks.com/question525.htm	4	48	49	41	46.0
	• http://en.wikipedia.org/wiki/Bit_stuffing	5	22	14	21	19.0

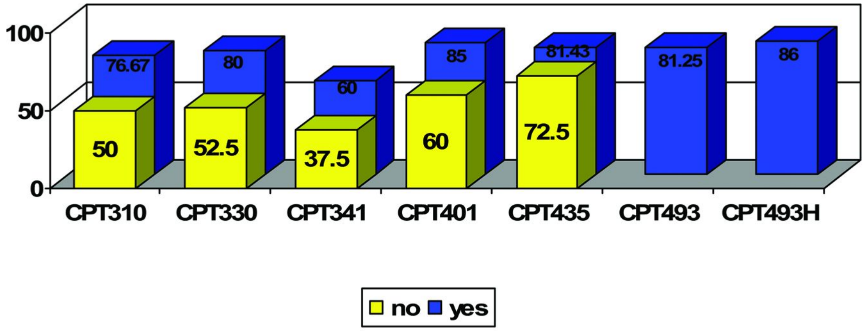

Figure 4. Exam Performance Comparison Utilizing CUBE System (Yes/Blue indicates students' exam grades using the CUBE learning system) (see color insert)

Table 5. Summary of research population and test results

CUBE System	**N Students**	Std Dev	Grade(Mean)	Min	Max	Std Error
No (Baseline group) ECET	37	20.68	50.0	0	90	3.40
No (Control Group) CPT	19	17.39	**53.68**	20	80	3.99
Yes (Treatment Group) CPT	34	11.27	**79.41**	40	100	1.93

5.4. Summary of ILE Research

The results of this research indicate the potential that Integrated Learning Environments have for improving both performance and knowledge comprehension. Integrating course materials that span a discipline by utilizing a Web-based tool allows students to be active participants in constructing meaning. Students utilizing the CUBE knowledge repository showed an average increase of 23.46 points in test scores on a standardized exam over students taking the conventional single course method. The combination of improved perceptions by the students of this approach and some reasonable quantitative improvement in test scores seem to indicate the potential of this approach

6.0. Emerging Technologies

A number of publishers, for example McMillan DynamicBooks (figure 5), provide tools to create dynamically linked text books with embedded audio and video. They also allow for a creative rearrangement of content to suit individual instructors. With the addition of enhanced collaboration and presentation tools such as Moodle, ItunesU and Second Life, to create a collaborative framework, the growth and evolution of e-Learning is assured. Refer to table 6 for examples of textbook publishers and the editing tools and links to those resources.

The initial e-Readers, Amazon's Kindle and Barns and Noble's Nook, have provided a starting point and shown the interest for eBooks in classrooms. The next generation of e-readers and tablets such as the IPAD, Dell and HP devices

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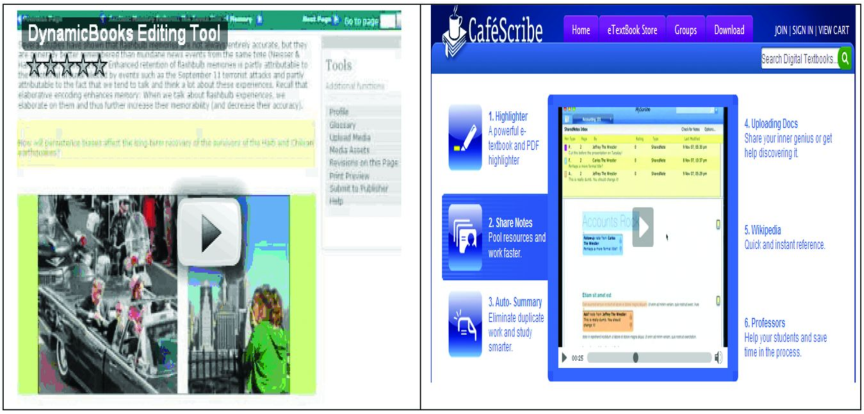
arriving in 2010, should allow for more complex integrated environments to be built.

The new generation of eBook editing tools allows instructors to reassemble textbooks and embed video, links to other eBooks and exams to dynamically evaluate student comprehension topic by topic." The modifiable eBook editions will be much cheaper than traditional print textbooks. *Psychology*, for example, which has a list price of $134.29 will sell for $48.76" (*23*). The general costs of eBooks are 30-40% of the cost of printed text books.

As of spring 2010 a number of colleges are selecting the second generation of devices, such as the Apple IPad, to be used as e-readers. The second generation devices add Web access that allows them to function as multipurpose devices and not simply as e-readers. Seton Hill University in Greensburg, Pennsylvania has announced that, beginning with the fall 2010 semester, every full-time student will get an IPad. New Jersey Institute of Technology is starting a pilot program, utilizing Apple's IPad, for fall 2010, where all text books for the Medical Informatics B.S. option will be provided as a comprehensive interconnected eBook package. This eBook IPad package will be cheaper than the purchase of conventional textbooks. As part of this pilot, the NJIT library has agreed to purchase eBook versions of these text books and will lend them out chapter by chapter for one month. The library software disables the book chapters after the allotted time frame. This library lending approach has been used successfully for the past year.


DynamicBooks Editing Tool
Best Page
Go to page
Tools
Profile
Glossary
Upload Media
Media Assets
Revisions on this Page
Print Preview
Submit to Publisher
Help
CaféScribe
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Search Digital Textbooks

1. Highlighter A powerful e-textbook and PDF highlighter
2. Share Notes Pool resources and work faster.
3. Auto- Summary Eliminate duplicate work and study smarter.
4. Uploading Docs Share your inner genius or get help discovering it.
5. Wikipedia Quick and instant reference.
6. Professors Help your students and save time in the process.

Figure 5. McMillan DynamicBooks and Follett CafeScribe eBook software. Composite illustration from: http://dynamicbooks.com/ and http://www.cafescribe.com/.

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Table 6. e^{2}Book editing tools

Company	*eBook editing software*
Follett	**CafeScribe** http://www.cafescribe.com/home/faculty.php Video available at this link illustrating features
McGraw Hill	**Create Software** http://create.mcgraw-hill.com/wordpress-mu/welcomeprimisuser/
McMillan Publishing	**DynamicBooks** http://dynamicbooks.com/
Pearson Education	**CourseSmart** http://www.coursesmart.com/instructors **• Video Tutorial** **• Distributes content from other publishers such as:** • Bedford, Freeman & Worth Publishing Group • Cengage Learning • CQ Press • Elsevier • F.A. Davis & Company • John Wiley & Sons • Jones & Bartlett Publishers • McGraw Hill Higher Education • Nelson Education • Pearson • Sage Publications • Sinauer Associates • Taylor & Francis • Wolters Kluwer Health
McGraw-Hill, Houghton Mifflin Harcourt, Pearson, and Kaplan Publishing.	**ScrollMotion** • Develop iPad eBooks for these Textbook Publishers http://www.scrollmotion.com/

Some of the core questions regarding eBook integration into universities are whether they will provide a quantifiable learning advantage, whether students and faculty will embrace them and what niche they will fill. Will these new devices replace existing PC's / Laptops or just be a new tool to augment existing technologies? Will students own both a PC for conventional processing tasks and a Tablet for portable environments? The migration to cloud computing seems to support the idea of owning only a lightweight, Web-enabled tablet as a front end to access software and databases in larger repositories. In addition evolving technology will make these tablet devices more capable blurring the boundaries.

One last concern is that, if information is stored in central repositories, it raises the fear of tampering. *"History is written by the victors,"* is a quote from Winston Churchill, who warned that diligence is necessary to ensure that information content is sacrosanct. This may require many parallel repositories, maintained by independent organizations, or a global United Nations style library. The book, Fahrenheit *451*, by Ray Bradbury, described a future where books were

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

burned and governments tried to control information. The population's solution was to memorize the books to ensure their continued survival. Another example is a short story by William Harrison, published in 1973, *Roller Ball Murder,* which illustrated one central world repository maintained by the five ruling corporations, similar to today's concept of "cloud computing,." In that story, the victors were able to rewrite or delete history. I am personally optimistic that with diligence our better angels will prevail.

7.0. Summary

Virtually all universities now offer e-learning courses that incorporate some level of interactive tools. The next step is to create interactive learning environments that actively involve students in learning and integrating information, initially within a discipline and later across fields. Tools are being developed to integrate and link concepts to provide a cohesive view of a discipline. Publishers and eBook developers have begun to actively join in the creation of more interactive environments. The number of knowledge repositories that link multiple disciplines is growing. The next evolution will link all of these components into a true integrated learning environment. Access to education and resources is still unavailable to many. The hope is that if information and learning resources become universal and Web access expanded, educational disparities may be resolved.

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Chapter 10

Good Animation: Pedagogy and Learning Theory in the Design and Use of Multimedia

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The chapter reviews some of the important guiding issues in the development of animations for educational purposes. Animation is situated as a tool in aid of visualization and the development of mental models. In this perspective, it is argued that animations that are designed for educational purposes should, along with the effort to develop new content knowledge, should also seek to enhance the internal models of the learner. It is argued that this can be best achieved by developing animations that are more explanatory rather than emergent or explorative. The choices made in the design of animations are informed by learning theories: Behaviorism, Cognitivism, and Situated Learning. A case is made for using animations in guided rather than open inquiry. Together with the principles of multimedia based on dual-coding theory, cognitive load theory, and schema development, a case is made for what constitutes appropriate design and use of animations in education. It is argued that good animation is one that abides by the research-based principles of multimedia learning, is designed with a mind towards a particular learning theory goal, is used in established protocols that target specific learning objectives, and is one that keeps in mind the possible end-use by the learner. Specific examples of design issues and how these may be resolved by a careful reading of learning theory is discussed. The Inductive Concept Construction (IC2) learning system and how it is guided by the principles of good media design and use is discussed.

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

Introduction

Issues in the Research on Animation as a Tool for Education

In this book, the tacit purpose for all the research effort and materials development in electronic media is improved learning. However, in designing and using animations, it is often easy to lose sight of that purpose and become caught up in the theoretical aspects and technical details of media development. For animation developers, the allure of creative expression, wrangling with and surmounting development and design issues can often make us lose sight of the goals for which these animations were initially developed. This can be further exacerbated when we see the deep student engagement with what we have wrought. User engagement with the design artifacts can easily—and falsely—be assumed to be a good indicator of engagement with content (*1–3*). Users, students and instructors, are easily enamored with artful details, bells-and-whistles, and again misinterpret engagement with material design as leading to better learning. While there is extensive research on the effect of different animation strategies on learning (*4–6*)—suggesting that animation techniques can have a strong impact on learning, there is also extensive data suggesting that it is the design elements within those animation techniques that strongly affect learning (*7–11*). In looking at the effect of animations on student learning, it is important to keep in mind that the observed results could well be an artifact of the multimedia design elements rather than the multimedia approach itself. These issues serve to reinforce the notion that we who develop animations and multimedia tools need to find a touchstone, a bedrock of research data, to guide our endeavors. In this article, we will look at the field of cognitive psychology and pedagogical theory to look for strong guidance into how animations for education purposes should be developed.

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Animation in Relation to Visualization

In as much as animations have many things in common with other visualization aids, animations have often been considered as a subset of the larger concept of visualization (*12*). Animation has often been used to further the goals of visualization. Likewise, animation has often been considered as one among the many tools in aid of visualization. It may be important to look at this intersection briefly to see if there is anything in visualization research that may help guide animation design.

Visualization can have two main meanings: external and internal visualization. We can imagine that the term *external visualization* can mean the physical manifestation of an idea, the physical expression of a concept. We can then choose to parse external visualization into many subsets: the many ways that cues—especially imagery—ably represent, realize, quantitative and qualitative data in a concise and organized fashion (*13*, *14*), and/or the many ways that information may be represented by a physically manipulable object or animation (*11*). We can choose to investigate the different levels of effects these may have on the learning of a concept (as, indeed, many have), but ultimately, what we are investigating is how these external visualization procedures, techniques, and tools come in aid of internal visualization—the ideas that a learner owns(*15*).

In this perspective, we shift the focus from what an expert provides to what the learner internalizes (and later expresses). *Internal visualization* is here taken to be the resultant mental representation or imagery derived from the given external visualization (*16*, *17*).

It would appear that the goal of visualization research—to provide effective external visualization tools and processes in order that a learner might develop properly expressed internal visualizations—is very much the goal of animation for education purposes. This is very much a cognitivist view wherein the goal of learning is to promote "expert rules" that are able to supply answers more completely and with more associations than "novice rules" (*18*) that will be discussed later in this article. We can take this a step further and state that, since "model" has been used interchangeably with internal visualization, it would appear that one of the more important goals of developing animations for education is to promote the development of "expert models" in the learner (*19*). It is therefore important to look at what our definitions of *model* are so that we can develop appropriate animations.

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Redefining Learning as the Development of Expert Models

If we so choose, *model*, as employed in science, can have a variety of meanings and serve a variety of educational purposes. Parsing *model* into its many forms can have the same purpose as syntactically analyzing the many forms of visualization as discussed in the previous section (*20*, *21*). As a community of scientists, we share an agreed upon representation of our conceptual knowledge: a *consensus* model. A consensus model is a shorthand description of what we, as a community, commonly hold and understand to be true. Such consensus models can be subdivided into *established* and *working* models. Established models are widely accepted expressions of readily agreed upon concepts. Working models are representations of premises or hypothesis and are used for the development of emergent knowledge. Established models can be further subdivided by purpose into *explanatory* models and *representational* models. The purpose of explanatory models is to quickly or concisely convey or ably support learning. In this sense an explanatory model need not contain the whole body of knowledge governed by that model. It is used simply so that learners may gain or develop a ready grasp of the objective or targeted concept. The purpose of representational models, on the other hand, is to express in a concise form a body of specific knowledge. In this sense, the objective of a representational model is less to act as a development tool for learning and more as a tool to convey knowledge.

In so far as we are interested in the promotion of learners, we have to try and access the student's *mental* models. Mental model, in this usage, is the individual learner's internal representation of his or her understanding of the body of knowledge. In Sweller's terminology, a mental model is the schema, the growing mental structures, developed from study and experience (*10*, *22*). This is very similar to the distinction made in the previous section between external and internal visualization in that we look at the way learners use and express explanatory and representational models so that we may gain access to their internal, mental models. As such, it is argued that the investigation on the different forms of modeling—and the animations we develop to support this—is important primarily so that we may better shape the learner's mental models, so that we can hope to develop expert schemata among our students (*9*).

In this syntactic analysis of *model*, we can argue that, while animations may be developed for all sorts of purposes, if we are developing animations for the purpose of education, for the purpose of guiding our students in the development of expert mental models, then we have to focus on our understanding of explanatory models. If so, then the effort to focus on what is explanatory from the perspective of the learner (as opposed to what the instructor or animation designer considers to be explanatory) means that we have to have an understanding of what learning is and what processes, mental and expressed, are involved in the development of expert models and schemata. We need to look at what the research in cognition has to say about the kinds of animations we produce.

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Implication from Cognitive Psychology Research

Behaviorism, Cognitivism (Constructivism), and Situated Learning

We can divide learning theory into three major schools of thought: behaviorism, cognitivism (*23*), and socially constructed or situated learning (*18*). Since each school of thought developed in response to the school prior to it, it is tempting to assume that the most recently developed learning theory is the most advanced. While different schools will argue for the primacy of their particular learning approach, it will be argued here that certain modes of teaching, learning, and assessment are appropriate depending entirely on the learning objective of a particular unit or lesson. As such, each school will be discussed in turn.

Behaviorism arose as a means of developing a readily analyzed form of learning (*18*). The learning theory was primarily as a response to the perception that an explanatory approach to mental science was erring on the side of argumentation and little data. Behaviorism was a rejection of expressing learning through a functional depiction of the inner, mental process, choosing instead to focus entirely on what was externally measureable. John Watson defined learning in measureable terms: if a learner were to encounter an issue requiring a response and achieved a resolution to that situation, and if on encountering that same or similar situation again the learner were to achieve a similar resolution in less time or with fewer steps or missteps, then it can be said that the learner has learned (*25*). Skinner responded to the contention that Watson's approach was entirely deterministic and explanatory only after the fact—a response could be explained based on some environmental stimulus only after the response to a stimulus was observed (and virtually anything in the environment could serve as a stimulus)—by refocusing learning as the change in the rate of response in order to achieve reinforcement (*26*). In Skinner's view a theory for learning was not absolutely necessary (*27*), learning could be defined as that which is measureable—the increasing response rate of a learner to bring about reinforcement. The use of flash cards, memorization tables (such as the multiplication table or in particular cases: the periodic table), question-response games, can be viewed as teaching processes that directly result from the behaviorist view of learning.

We can then imagine that if animations were to be used to promote behaviorist goals, we would develop drills and skills development animations that help promote algorithmic thinking, pattern recognition, and speed. For example, arcade style games that challenge the learner to complete certain tasks faster and with fewer errors (errors being negatively reinforced) (*28*) take on a behaviorist approach to learning. Similarly, textbook exercises whether guided or simply matching answers to a databank also take on a behaviorist view of learning (*29*).

Cognitivism rose to prominence partially in response to the perceived limitations of the behaviorist view of learning. Chomsky (*30*), for example, argued that while behaviorists could achieve rigor in a laboratory setting, there was simply no way of maintaining that rigor outside the laboratory. Moreover, there was a difficulty in extrapolating learned behavior to situations outside the laboratory. Jerome Bruner redefined learning as “concept attainment” (*31*). This can be viewed as the development—independent of rate—of expert rules. As such, Bruner could still study learning in an objective way if access to the learner-developed rules could be achieved. Thus, the definition of learning shifted from getting the correct answer and how fast the correct answer was obtained, to using the correct method of getting to the answer (*32*). In so far as the constructivist view of learning focuses on how the learner acquires and develops expert rules, it will be considered in this discussion as an offshoot or an extension of the cognitivist view of learning. Processes that emphasize concept construction such as the development of concept maps (*33*); the emphasis of Everyday Mathematics (*34*) on multiple processes, spiraling skills, and understanding processes rather than being expert in a specific algorithm or behavior; the study by Nakleh *et al.* (*35*, *36*) that showed that students were more able to answer algorithm-based problems as opposed to those that emphasized concepts are all predicated on a cognitivist view of learning.

If we were to develop animations with the objective of developing schema construction, we might develop simulations that allow the learner to develop their own interpretation of the phenomenon—with or without guidance. The many animations that provide simulations of chemical and physical phenomena such as the PhET series (*37*), NetLogo (*38*), and Connected Chemistry (*39*), or simulations that require the student to develop their own understanding (*40*) implicitly practice the cognitivist view of learning.

Situated Learning rose in response to both the behaviorist and cognitivist view of learning arguing that neither approach considered the possibility of learning occurring outside the studied environment. Neither view considered what the learner brought to the situation, the context in which a learner viewed a learning situation, and what the learner is attempting to achieve—goals which may be different from the instructor-stated or predetermined learning objectives (*41*). Vygotsky (*42*) put forth the idea of “zone of proximal development” as the line between what a learner can do alone and what the learner can do only with assistance or guidance by higher-level learners. As such, learning can be considered as moving this line forward in context to what the learner perceives his or her role to be in a community activity. Lave emphasized the idea of

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learning as a process akin to apprenticeship (*43*). As such, learning was not an activity that a teacher imparts to a student, and neither was it an activity that occurred solely within the learner. Learning was something achieved as a community and which did not reside solely in either teacher or student; both learn in this process. Processes that have had some impact in the learning of chemistry such as Process-Oriented Guided-Inquiry Learning (*44*) and Peer-Led Team Learning (*45*) owe much to the idea of situated learning. The idea here is that the learning goals of the student are addressed equally as the learning goals set by the curriculum or the instructor. Moreover, the knowledge developed in such processes is developed through the dynamics of cooperative learning, one in which the individual students' learning goals become apparent and addressed by the peer-to-peer activity.

If animations are to be used for goals that are best defined as situated learning, then the animations have to be made in conjunction with the expected usage of such animations, especially if this involves cooperative learning activities with contextual cues. In this perspective the animation that we provide is but one of the components that promote learning. Learning happens as a result of responding to the prompts of the provided animation and the way those responses are scaffolded (*51*) in our instruction protocols (*52*, *53*).

While certain learning processes achieve prominence, become adopted, or become in vogue, it is argued here that each of the learning perspectives described previously in its own time produced research results that were accepted and contributed to learning theory. The rise of a particular learning theory to some level of prominence does not necessarily negate the results obtained in the investigation of a previously developed system, it merely forces us to consider the parameters by which the previous system's results were obtained and are still effective. As such, it is argued here that all these processes hold some merit and the teaching/learning processes that we employ should largely depend on the stated objectives of the lesson or unit. If the objective is to have a student rapidly complete a multiplication calculation, then it might be best to achieve that goal by a strict stimulus-response memorization technique. A behaviorist approach or perspective is germane to this learning goal. If on the other hand, the objective is to understand the process by which a distance stated in miles may be translated to time of travel or how many physical steps are needed to be made, then perhaps, expert rules need to be learned. A cognitivist perspective is important in this case. And certainly, either process can be promoted with the aid of a learning community and in the context of the individual learner's goals.

If we consider the fact that only 5% of the students in high school consider science careers (*54*), we can clearly see why there has been a push for secondary science curricula in the context of societal issues and citizenship (*55*, *56*). It could then be argued that science as a learning community should be a prominent learning process and much can be learned from a situated learning perspective. The argument that contextual learning is extant whether we perceive our learning goals to be that which may be readily achieved through a situated perspective of learning or not requires the animation developer to consider how the animation is used in practice. Thus, while we ought to develop animations for an express learning purpose, whether it is the quick-response rate of behaviorism or the development

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of expert internal models of the cognitivist, we have to keep in mind how we expect these animations will ultimately find its use with the learner. The learner-defined usage will ultimately control the effectiveness of the animation.

The Case for Guided-Inquiry

Inquiry learning processes in its many forms: discovery, case-based learning, problem-based learning, etc., (*57*) may be considered as learning protocols that have risen from the constructivist point of view (*10*). In this approach, part of the duties of the educator or animation developer was to provide a learning environment or situation in which a learner, either through individual effort or as part of a cooperative learning process, might be able to develop his or her own conception of the targeted learning objective. The inquiry premise stems from the constructivist view that, since all knowledge is constructed by learners, direct instruction is not an effective method to achieve constructivist goals and an effective educational form is that in which learners have been given the opportunity to develop the concept for themselves. This means that educators should provide the learning environment, situation, or context, some minimal and necessary guidance, and allow the learner the freedom to state the learning objectives, the investigative and learning protocols, and the form of the expression of the conclusions and knowledge (*58*, *59*). In effect, students in inquiry-learning were expected to develop the "expert rules" or expert internal models through an essentially self-guided process.

Inquiry learning processes have risen to prominence. Both the American Chemical Society (ACS) and the National Science Teachers Association (NSTA) promoted inquiry-learning as a central requirement in science education in their position papers (*56*, *60*). The supposed effectiveness of inquiry learning processes, especially in science-learning, came about partly because there was an easily perceived symmetry between the investigative scientific process and the inquiry-learning process (*61*). In its extreme implementations, the open inquiry learning process involved learning through an experiential protocol, one in which the learner underwent the research processes of the discipline in the effort to learn a targeted learning objective (*62*), or where the students were required to devise their own solutions to real and contextual problems (*63*). The implication was that the acquisition of expert rules was interfered with by the intervention and guidance of the instructor.

However, there is an on-going debate whether this adaptation of constructivist theories into inquiry-learning protocols have had a positive impact in student performance (*64*, *65*). It is argued that there is very little data supporting a completely unguided or minimally guided, open inquiry. Moreover, the expectation that a novice learner, with a limited long term and working memory, might be able to emulate the investigative process of an expert researcher runs counter to the current theories of cognitive architecture. The way an expert does research in order to gain new knowledge is not at all similar to the way that same expert learns established knowledge (*62*).

On the other hand, there is a growing body of evidence in support of guided-inquiry as opposed to open inquiry (*66*–*69*). The premise here is that, unlike in

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an open inquiry process, students are never completely left alone to glean expert rules from a prepared activity. Rather, the prepared activity is only the starting point for further guidance in which the student is still expected to develop expert rules. Moreover, these rules are continuously checked against those of their peers or by the attending expert. Guided-inquiry, in this respect, recalls the zone of proximal development put forth by Vygotsky and places the instructor in the role of a master to an apprentice. The educator was placed in the position of developing or producing situations and protocols designed to find the student's zone of proximal development and promoted behaviors that allowed the student to grow that zone. When this process was done in conjunction in the context of a group or cooperative learning, guided-inquiry could be viewed as a merging of constructivist principles with situated learning protocols (*70*).

Animations can be categorized depending on the teaching principles that have been adopted into their design. These principles can range from direct instruction to open inquiry. Animations that are meant for direct instruction usually provide content in an essentially linear fashion, very much like a video, and interactivity, at best, is predicated on a self-guided navigation of the content (*71*). Such animations are used primarily to deliver information in what is considered to be an engaging manner. On the other end of the spectrum, open inquiry animations provide little guidance or cues as to what the learning objective might be, and the learner is expected to extract knowledge by a careful study of the manipulable variables on screen (*37*, *38*). These animations expect the learner to develop a schema without intervention from the developer or instructor. Extreme examples of these animations do not even contain cues for the learner, suggesting that the designers did not want to direct the learner toward particular learning goals. These animations tend to raise issues regarding the suitability of the inquiry process to science learning. In between these two extremes are the animations developed with the experience of the educator regarding the zone of proximal development or the level of mental development (*72*) of the average student. As such, guidance is provided so that a student may, with the help of his or her peers or attending educator, learn the target lesson; the student is neither left alone to develop the knowledge (as in an open inquiry) nor is the knowledge completely digested for the student (as in direct instruction).

If the research on learning correctly point out that a guided-inquiry approach scaffolded by a constructivist/cognitivist perspective is one of the most effective forms of teaching, then we who design animations have to tailor our products for this specific protocol. It would mean that we would choose to target the development of expert internal visualization, expert mental models, using explanatory models in the context of the expected or observed zone of proximal development of our students and in a cooperative, guided-inquiry learning environment. Specific examples that exhibit how animations may be designed for the purpose of guided-inquiry will be given in subsequent sections.

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Choices in Animation Design for Chemistry Education

Animations and the Learning Domains of Chemistry

Johnstone's depiction of the chemistry ontology as being comprised of three interacting learning domains: macroscopic phenomena, symbolic representation, and particulate conception (*73*) has directed much education research into determining how students think and how educators teach relative to these domains. It is clear that much work has to be done in order to improve the abilities of both students and educators to think along these three learning domains. Investigations have shown that many students cannot show mastery of chemistry concepts in all three domains (*74*, *75*). This lack of expertise extends even to teachers (*76*, *77*).

There is a growing body of evidence suggesting that multimedia learning, simulations, and/or animations may strongly increase students' abilities to make connections between these three learning domains (*78–83*). Students who have been shown some form of multimedia representation of physical or chemical concepts are more able to include expert models in their description of such phenomena then students who were given only a one domain explanation or who were given explanations that did not involve some form of multimedia presentation.

Some Decisions To Be Made in Animation Design for Chemistry Education

Despite the established positive effect of animations across the chemistry learning domains, educators still wrestle with a multitude of options when they attempt to develop animations with the goal of educating general chemistry students. Issues related to accessibility: font size and font styles, close-captioning for the hearing-impaired, color palette for the visually-impaired, design of recognizable icons and buttons, screen size and resolutions, narration speed, *etc.* are daunting enough, but when these are placed on top of the goal of having students learn chemistry concepts, then the issues become even more complex. A recent report in the ACS Committee on Computers in Chemical Education (CCCE) online conference (*84*) exemplifies some of the very specific questions an animations developer might have to deal with in the context of chemical education. Being that chemistry phenomena are dynamic and complex, how much of this dynamism and complexity should be incorporated in the animations? Should the particle motion depict what it is in reality (as experts understand it) or should we slow it down for clarity purposes? How much interactivity should be incorporated in the animations? How much of the animations should be generated by the learners themselves? The range of questions that a designer has to grapple with can get into such fine detail as should atoms be depicted as solid or "fuzzy" spheres. We quickly get into situations where these questions are answered, perhaps unfortunately, using the designer's instincts or personal preferences.

In so far as the animations are meant to be used for education purposes, for developing expert internal models, to promote expert schema, then it is argued that such questions should be couched in terms of how these animations can best promote student learning. This section attempts to restate the preceding questions in the language of cognitive psychology in the hope of better answering them.

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Should animations be in the service of established models or should they be working models? This is a question of audience. If our audiences are high school or college students who are learning foundational concepts, then animations should provide access to established models. Animations depicting working models should be reserved for research purposes. This does raise the question of how much emergent knowledge should be incorporated in animations, and this part of the debate goes to the question of how much guidance should be provided in an inquiry process. Taking into consideration the increasing evidence that full, open inquiry processes do not work, and the idea that we, educators, should be aware of our students' zone of proximal development, then it can be argued that a guided-inquiry process is best suited for learners, and that animations should be developed so that students can construct their own schemata (which they will do anyway). As such, animations in the service of education should neither be developed to be some kind of direct instruction nor should they be provided with no or minimal guidance.

Should animations depict explanatory models or representational models? Again, the question goes to purpose and how best to achieve that purpose. An educator and animation designer must answer the question of whether a fully representational animation could be too complex to be understandable without much guidance. The answer seems to be, as was discussed in the section on inquiry, that guidance is necessary and an awareness of the learners' zone of proximal development is necessary in order to optimize the level of guidance. A fully representational animation could require more guidance from the instructor as to defeat the process of guided inquiry. The principles of coherence and signaling (discussed in the section following) also seem to suggest that the animation be reduced to essentials with cues. It may not be possible to have both accurate depictions of reality as we know it and also have a minimalist representation in order to achieve the learning objectives (*85*).

The Principles of Multimedia Learning as Best Practices

Design parameters in the development of multimedia materials are available. Mayer's research has led to the development of a set of principles, which can stand for a best-practices outline of what constitutes good multimedia design (*7*, *8*). These principles were derived from Sweller's Cognitive Load Theories and Paivio's Dual-coding Theory. Studies on cognition have shown that learners accept and store information through visual and auditory channels (*92*, *93*). It has been shown that the learner's ability to construct conceptual relationships, schema, can be impaired if the information is received through only one of these channels and the learner is required to store much of the received information in short-term, working memory (*9*, *10*). It can be argued that textbook reading relies heavily on the visual channel, while a traditional lecture relies primarily on the auditory channel. If this is so, then it is possible to cognitively overload these channels and learning becomes impaired (*94*). It is therefore useful to investigate whether other modes of content delivery can be provided in which the auditory and visual channels work to complement and supplement each other to enhance learning.

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

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The first seven of these principles have ample supporting evidence, and correlates well with the findings of other researchers (*1*, *4–6*, *95–97*). The final three have some preliminary evidence and is beginning to be scrutinized more deeply by the education community. In so far as these principles are supported by research data from different research groups, it is imperative that we, who design animations and multimedia experiences for education purposes, adhere to them as much as possible and incorporate them in our design considerations. The *Multimedia Principle*: multimedia in this context is any delivery of information using the dual modes of visual and aural sensory inputs, and it states that students learn better when both sensory channels are used to deliver the learning experience. Corollary to this and in keeping with the dual sensory input, the *Modality Principle* emphasizes that students learn better when the words in a multimedia message are presented as narrated text rather than printed text. If printed text is used alongside the images supplied, the *Spatial Contiguity Principle* suggests that multimedia-learning experiences that are designed so that corresponding words and pictures are presented near each other provide a better learning experience than when those text and images are far apart. Similar to the spatial contiguity principle and in effect when there is narrated text, the *Temporal Contiguity Principle* states that students learn better when a multimedia experience is designed so that the narrated text are supplied simultaneously to the provided image. The *Coherence Principle* states that learning is hurt when interesting but irrelevant words, pictures, sounds, or music are added to a multimedia presentation. The *Redundancy Principle* states that multimedia designed with narration should not have the narrated text also in print. The *Individual Difference Principle* states that design effects are stronger for low-knowledge learners than for high-knowledge learners, and for high-spatial learners than for low-spatial learners. There is some data in support of the *Personalization Principle*, which suggests that a conversational presentation style is better than an expository style. Likewise, there is a growing body of evidence suggesting that the *Interactivity Principle*, that students learn more deeply when they are in control of the presentation rate, is true. Data also suggests that students learn more deeply when hints to the learning objectives or learning pathway are provided with the multimedia experience and this has been tentatively called the *Signaling Principle*.

Mayer’s research and the growing research body that support and corroborate it strongly suggest that there are appropriate animation design parameters that have to be employed if we wish to develop effective animations for education purposes. It seems that animators now have a solid touchstone in design. If we couple this with what is known in learning theory, we also have a solid foundation for animations use. The last section of this article will look at the author’s effort to prepare and use animations according to these guidelines.

The Inductive Concept Construction (IC2) Learning System(*98*)

A learning system: the Inductive Concept Construction (IC2, pronounced "I See Too") learning system was developed (2002-2004) and tested (2005-2008) among the General Chemistry students of the University of Texas-Pan American (UTPA) in Edinburg, TX. The IC2 system had three major components: an electronic textbook (eBook) made entirely using Adobe's (then Macromedia) Flash animation authoring software (*99*), an out-of-the-lecture hall cooperative learning system (*100*), and a formalized formative classroom assessment (*101*). Students were expected to go through the eBook animations, discuss the material using the guides and cues provided in the eBook and the accompanying hand-outs that were provided through Web-CT (now Blackboard) (*102*), and then express their learning gains in a highly formalized formative assessment protocol in the classroom. Using this learning system increased the concept learning and transfer abilities of the students well above those who received traditional direct instructions.

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eBook Design Issues

Mayer's multimedia learning principles were observed whenever and as much as possible. Visuals and narrations were always used (Multimedia Principle), text was only used for symbolic references and learning guides—narrations were used most of the time (Modality Principle), active animations were kept to certain parts of the screen to allow focus on the action (Spatial Contiguity Principle), and narrations were timed to the animation action (Temporal Contiguity Principle). Extraneous animations and text were kept to a minimum. Sidebars were hidden and accessible only by a button-click (Coherence Principle). Control of the animation was given to the viewer through the normal pause, rewind, skip-forward buttons, as well as manipulable virtual objects and buttons on the active screen (Interactivity Principle). Visual, verbal, and contextual cues were provided to guide the students through all the animations (Signaling Principle). These included simple beeps to signal an end of a section, arrows to point out important aspects of an animation, pauses when the student was expected to take time to inspect an animation, symbolic "magnifying glass" to focus in on an animation aspect, etc.

Some of these design elements may be seen in figure 1. The screenshot was taken during the sequence wherein key features of the particular animation was being described, in this case the "magnifying glass" which "showed" the gas particles above and below a chamber with a movable piston and enclosing an ideal gas. Normally, the default setting for the close-captioning system is set to *off*—in order to adhere to the proscription of the Coherence and Redundancy principles. For this screenshot, the captioning was turned on and it can be seen in figure 1, label 1, that the scrolling text in the strip near the bottom of the screen is timed to the narration (Temporal Contiguity Principle), and is also timed to the animation of the arrows pointing to the gas particles above the piston (label 2). At this point, in adherence to the Spatial Contiguity Principle, while there are elements already on the screen, the focus of the viewer is drawn to the arrows (label 2) that are describing the gas particles in the atmosphere above the piston both in the macroscopic and particulate simulation. Allowing for the Interactivity Principle, the narration and animation may be paused and continued at any time (label 3), and in this particular simulation, the elements of the apparatus: the pump (label 4), the thermal jacket (label 5), and piston clip (label 6), will be manipulable after the brief introduction of each element. Apart from being able to manipulate the simulated gas apparatus, additional cues (Signaling Principle) are provided through a "guide table", in this case, a list of suggestions on what the user might want to investigate (label 7). While this particular screenshot contains many elements, each of these elements are introduced slowly and on an as needed basis in order to minimize the additional cognitive burden of learning the simulation conceit.

Other design issues predicated on accessibility were also incorporated into the over-all design of the eBook modules. Careful attention was made on font sizes and colors and the use of serif versus san-serif fonts—making sure that there was a consistency in font as a matter of the text function. Main titles and important text were usually in yellow sans serif font, subtitles in white sans serif font, standard body text were in white serif font, etc. A color palette was used to emphasize contrast to ensure readability for students with poor color acuity. A dark background was used with bright text. Animations colors were colors were also chosen to provide the best contrast.

Throughout the eBook, a strong connection between the three learning domains of chemistry was made apparent to the student. These learning domains were provided sequentially as sections to a learning unit or module (in the author's view, Johnstone had never intended that these learning domains be *simultaneously* imparted to the student). Thus, in the IC2 eBook for example, a simulation on the macroscopic phenomena of gases (the macroscopic phenomenon simulator is shown in part in figure 1, label 8) was provided in the first section of the Ideal Gas module, followed by a section on the same macroscopic simulator but with a side animation of the particulate conception of the phenomena (figure 1, label 9), and finally a discussion of the symbolic representation and calculations in Ideal Gas Law. This was then rounded with a concept presentation of the Kinetic Molecular Theory. All these different chemistry learning domains: the macroscopic, the particulate, and the symbolic, were treated in separate sections. However each section could be accessed through the menu system (figure 1, label 10) at any time and from anywhere in a particular section, and there were many instances where the different learning domains were present even if the focus of the treatment would be on one specific domain. As such very little effort was made to control or study the sequence of the treatment of each domain.

The explanatory models used for the eBook were tailored to the estimated (*103*) zone of proximal development of the students at UTPA. As such very seldom was a representational model used. Atoms were depicted as solid spheres when no gains were expected by using "fuzzy" electron cloud depictions. Molecular vibrations and bond rotations were seldom included when only the translation and rotation of molecules were considered relevant to the discussion (such as in solution formation). Molecules were represented as single spheres when the internal structure of the molecule was not germane to the discussion.

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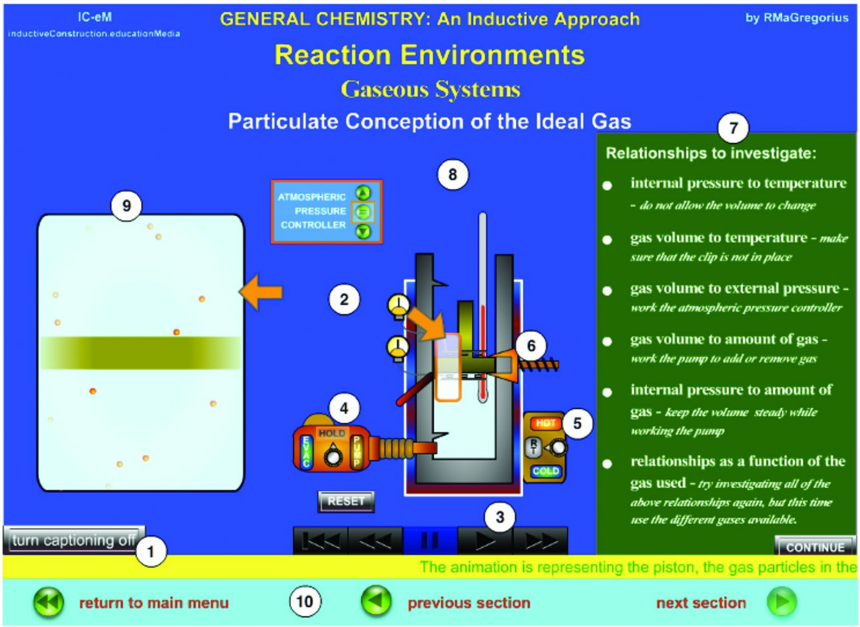
IC-eM
inductiveConstruction.educationMedia
GENERAL CHEMISTRY: An Inductive Approach
by RMaGregorius
Reaction Environments
Gaseous Systems
Particulate Conception of the Ideal Gas
ATMOSPHERIC PRESSURE CONTROLLER
HOLD
EVAC
PUMP
HOT
COLD
RT
RESET
turn captioning off
CONTINUE
return to main menu
previous section
next section
1
2
3
4
5
6
7
8
9
10

Relationships to investigate:

- internal pressure to temperature - *do not allow the volume to change*
- gas volume to temperature - *make sure that the clip is not in place*
- gas volume to external pressure - *work the atmospheric pressure controller*
- gas volume to amount of gas - *work the pump to add or remove gas*
- internal pressure to amount of gas - *keep the volume steady while working the pump*
- relationships as a function of the gas used - *try investigating all of the above relationships again, but this time use the different gases available.*

The animation is representing the piston, the gas particles in the

Figure 1. A screenshot (with labels added) from one of the modules in the IC2 eBook.

The principles that could not be strictly followed were the Redundancy and Personalization principles. Since an adjustment for students with hearing impairments or difficulties with the English language (85% of the students at UTPA were of Hispanic backgrounds, many of whom still lived in Mexico or were first or second generation Americans whose first language was not English), close-captioning, a running text at the bottom of the screen timed to the voiced narration was considered necessary (figure 1, label 1). In order to allow for the Redundancy Principle, this option's default setting was set to "off". Likewise, since familiarization with technical terms and discipline specific jargon was a goal in General Chemistry, the Personalization Principle could not be strictly followed.

As suggested in the previous section on learning theories, the eBook animations were designed to fit a particular learning theory perspective. In cases where the students were expected to develop the concepts for themselves—such as the macroscopic phenomena and particulate conception of the Ideal Gas Law, guided simulations were provided (*40*). This was in keeping with a constructivist view of concept learning and expert rules/models development. In cases where the targeted learning objective was deemed well in advance of what the average student could learn without significant guidance—as based on the informal assessment of the average students' zone of proximal learning—and/or the students were simply expected to extract information from data (only minor or tangential gains were expected from a simulated collection of data), and/or no appropriate simulation was available that would guide the students to the targeted concept—such as in the case of entropy or the Schrödinger model of the atom, animations that had a strong guided component, very close to being direct instruction were provided (*104*). In cases where a straightforward rote memorization was required or expected, such as in the case of binary inorganic compound nomenclature, or algorithmic problem solving, drilling exercises and/or arcade-style games were provided (*28*, *29*). In such cases, a behaviorist perspective was taken, no conceptual learning was expected, and only the rate of response was considered important. As such, the eBook modules were specifically tailored to the learning objective (whether behaviorist or constructivist), and delivered with some idea of the zone of proximal and mental development of the average student in UTPA.

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Out-of-the-Lecture Hall Cooperative Learning

The class (average size: 75) was split into groups of six students (*105*). Students were expected to meet outside of the class period and out of the lecture hall to discuss the upcoming lesson. Calendars, learning guides and questions, forums, and quizzes were provided prior to the classroom discussion and were delivered through Web-CT. Although the cooperative learning scheme was not strictly enforced or monitored, students reported on surveys that they took this seriously and was necessary in order to prepare for the upcoming classroom formative assessment. In the experience of the author, the groups usually met in the two hours prior to the class meeting, most of the students were observed occupying the UTPA library meeting rooms in the two hours prior to class.

Implementation in the Classroom

It is important at this point to emphasize that no classroom lectures or direct instruction were used in the IC2 system for the entire General Chemistry program. Classroom time was taken up by a formal formative assessment process. This was done to further emphasize the socially constructed learning aspects of the learning system and to drive home to the students that the any derived concepts would come from the students' own study of the eBook and during the out-of-the-lecture hall cooperative learning process. The formal formative assessment in the classroom followed the following pattern: (1) a question was assigned at random to each group, a second set of questions were shown on a projection screen, (2) the groups were given fifteen minutes to discuss their question and the questions that were shown on screen, (3) a random member of the group was asked to answer their assigned question, another member of a group, also chosen at random, would be asked to answer one of the questions on the projection screen, (4) both steps 2 and 3, would be followed with a randomly chosen member of a different group being asked to critique the answer provided, (5) a consensus answer would be formulated and written on the board. The sequence of questions was designed to develop the day's lesson so that at the end of the series of questions a learning objective will have been discussed.

All answers were modeled and exemplified for the students. Questions that focused on concepts were required to be answered with: (a) a single thesis statement, (b) an exemplification of the thesis statement, and (c) additional examples if necessary. Questions that required a mathematical resolution were required to be answered by: (a) stating the mathematical equation, (b) explaining the different symbols of the mathematical equation, (c) rewriting or reformulating the mathematical expression as necessary, (d) plugging-in the data, (e) stating the answer. Critiques were likewise formalized. Critiques of concept questions were required to have the following components as necessary: (a) a summary of the answer provided, (b) a statement of any perceived missing arguments or ideas, (c) a statement of any misconceptions in the answer, (d) a statement of possible better examples or expressions of the answer. Critiques of algorithm-based questions included: (a) a description of why the answer made sense (or did not make sense), (b) any possible variations in the approach. All answers were graded either individually (critiques) or as a group (concept and algorithm questions). A tabulation of recitation grades was provided in the returned mid-term examinations.

In this process, the instructor only interjected when a misconception was present and not corrected for in the answer and critique. All learning statements (those that were written on the board) were arrived at by consensus. The instructor made sure that none of these were a result of direct instruction or content delivery from the instructor.

Keeping this process formal ensured a steady flow of the discussion so that all the required material in the semester was covered properly and adequately. Forcing the students to express their understanding made their knowledge not only apparent to the instructor but to the students themselves. The peer-peer discussion, both in the cooperative out-of-the-lecture hall discussion and in the in-class formative assessment, was in keeping with a situated or contextual learning philosophy. Although the learning guides did direct the students to particular learning objectives, the discussion allowed for students to bring their concerns and prior knowledge to the fore. The formal answer and critique allowed for students to assess their own level of knowledge in relation to their peers.

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Results (*106*)

A survey of student attitudes toward the IC2 learning system showed that, after the first 2-3 weeks of class, students were overwhelmingly in favor of this learning system over the traditional textbook and direct classroom instruction. This was corroborated by the individual interviews conducted. Students did suggest missing an “authority figure” who would corroborate or confirm their prepared answers—suggesting that students were still aware that their learning would eventually be tested in a standardized test and their grades were dependent on this. The students were well aware that a traditional textbook could not ably replace the eBook. They were also aware that any single component of the IC2 learning system, taken separately, would not provide the learning they gained in going through the entire system. Most students believed that their learning gains in the IC2 system were higher, their performance on tests far better, than if they had gone through the traditional teaching system (*52*, *107*, *108*).

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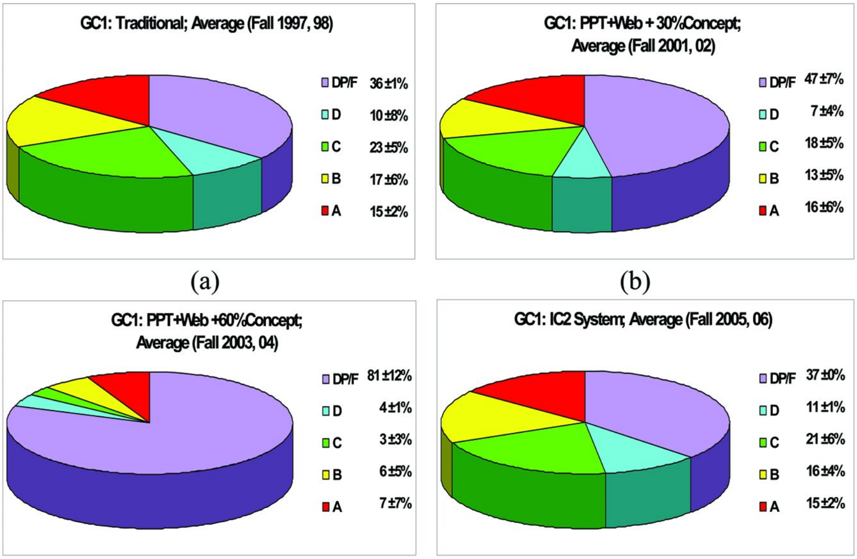

(a) (b)

(c) (d)

Figure 2. Grade distributions for various learning protocols.

A comparison of student performance of students in the IC2 learning system to students who received traditional textbook and lecture-based instruction or those who received the traditional lecture augmented by electronic notes and WebCT support showed an overwhelmingly better performance for students in the IC2 system (figure 2). Figure 2a shows a typical grade distribution at the study institution for students receiving traditional instruction using printed textbooks and lectures. Figure 2b shows the impact of changing 30% of the test questions to concept questions, and figure 2c to 60% concept questions. These were the results despite an effort to augment the classroom instruction with PowerPoint lecture notes and Web course tools support such as online quizzes and assignments, calendars, online asynchronous tutorials, etc. The results were not changed by efforts to adjust or modify the lectures to be more focused on concept learning. Figure 2d shows the effect of switching to the IC2 learning system—this despite a 60% concept question test/quizzes. The scores were consistent over several years of course offerings (*109*).

Summary

There now exist sufficient guides both in media development, education, and cognitive psychology research to support well-designed and effective animations for learning purposes. Mayer's research in multimedia learning provides animation developers a very good set of best practices principles for effective electronic media materials for education. It is important to accept that the educational effectiveness of a prepared animation cannot be separated from the way these animations will be ultimately used by the learner. An understanding of the educational goals as related to theories in cognition, learner generated internal models, and visualization, provide a strong scaffolding to develop truly effective animations for education. An understanding of how these animations would be used by the students and incorporating this in the animation design would make for an effective learning experience. It is hoped that the treatment here and elsewhere of the IC2 learning system has shown that well-developed animations can be guided by learning theory and can be used in the production of teaching and learning protocols that have a better chance of improving student performance over teaching protocols based on static, printed textbooks and direct instruction.

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15. While we could also consider the learner's expression of their internal visualizations as "external visualization", and while it is important to understand the mechanism by which the learner manifest his or her ideas, these are well beyond the scope of this discussion. The author will take the stance here of phenomenology: only the learner's expression of their internal visualization can be accessed and discussed and the quality of the learner's manifested internal visualization is a direct indicator of the internal visualization itself.
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Chapter 11

Reaction Explorer:Towards a Knowledge Map of Organic Chemistry To Support Dynamic Assessment and Personalized Instruction

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Computer-based learning systems enable interactive learning opportunities that are not possible in a traditional teaching setting. We have previously developed Reaction Explorer an interactive tutorial system for organic chemistry, synthesis, and mechanisms at the college level. The tutorial is powered by an underlying organic chemistry expert system comprising over 1,500 reaction rules, allowing it to generate a virtually infinite collection of problems, and has been used by students at our University for the past three years. The work presented here seeks to develop novel intelligent modules to optimize and personalize student learning trajectories by monitoring each step in a student's progress and learning to propose optimal individualized problems that are at the boundary of a student's knowledge. Specifically, the system is being upgraded with modules for computer-based dynamic assessment and personalized instruction based on concepts from the theory of knowledge spaces.

By performing statistical data mining on historical problem completion data, a knowledge map for organic chemistry topics is constructed to specify the dependencies of learning points. This knowledge map enables dynamic assessment where the system can rapidly and precisely model a user's knowledge state. Finally, models of individual user knowledge states allow the system to optimize learning trajectories by preferentially selecting user practice problems that are neither "too hard" nor "too easy" for the individual user. While various optimizations and validation experiments must be completed to increase confidence in these new functionalities, the methods described here and implemented in the system are laying the groundwork and infrastructure to make dynamic assessment and personalized instruction possible for the complex subject domain of reactions in organic chemistry.

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1. Background

Computer-based learning systems enable interactive learning opportunities that are not possible in a traditional teaching setting based on group instruction and paper-based assignments and examinations. Compared to paper-based instruction methods, computer-based learning systems provide many direct benefits including immediate feedback for students, and automated grading support for instructors. Within the subject domain of chemistry, several online learning systems have already provided some of these benefits to students and instructors, including ACEOrganic (*1*), LON-CAPA (*2*), MCWeb (*3*), OWL (*4*), WE_LEARN (*5*), and WebAssign (*6*), but significant opportunities for improvement remain for online instruction in organic chemistry. More recently, the Reaction Explorer tutorial system (*7*) has further advanced the instruction opportunities by building a learning system atop a reaction prediction expert system instead of relying upon a fixed set of pre-constructed problems. This underlying prediction engine allows the Reaction Explorer system to generate a virtually limitless number of organic chemistry problems for students to work on, including the most challenging and open-ended problem types (multi-step synthesis and mechanisms). Furthermore, the system offers students specific feedback and predictions for any reactions they input as possible problem answers, even to the point of allowing open-ended virtual experiments to support student inquiry-based learning (*8*).

While the Reaction Explorer system can generate a virtually limitless number of problems, offering students unlimited "replay" value, no individual student is expected to attempt millions or even thousands of generated practice problems. In current usage, students are instead assigned to complete a minimum number of problems (typically 5 to 10 per week) from a random sample of system-generated problems. The sampling is not entirely random as students can guide the process by selecting which "chapters" of subject content the generated problems are based on. Ideally, students will select subject areas that cover a range of material they need to learn, practice, and improve upon. In practice however, many students seek out easy subject topics as the fastest means to complete the minimum assigned requirements. Even if students did legitimately attempt to select for topics they need practice in, self-diagnosis of proficiency is unlikely to be reliable.

The work presented here seeks to optimize student learning trajectories by giving them the "most useful" problems to work on instead of choosing problems at random. Of course, the definition and identity of which problems are "most useful" is a highly individualized, student-specific attribute. Rather than try to designate questions that are "most useful overall" across the aggregate of all students or have students attempt to self-diagnose and self-select subject topics, a goal of greater precision is to automatically identify the individual needs of each student and develop problem sets personalized for them. Decades of research have shown that for a given individual, the most useful and enjoyable problems are those precisely situated at the very fringe of an individual's current knowledge, corresponding to problems that are challenging, but not too easy nor too hard. Thus, being able to accurately estimate the fringe of a user's knowledge is essential in order to optimize both his learning trajectory and learning experience.

1.1. Knowledge Space Theory and Applications

To achieve the desired properties described above, we can build upon many principles established in the theory of knowledge spaces (*9*). This theory has been successfully applied in other domains (see for instance the ALEKS system (*10*)). Knowledge spaces provide a theoretical framework for precisely assessing an individual's knowledge of a subject domain and inferring learning dependency orders that indicate what material each individual is best prepared to learn next. Several relevant concepts from this theory are defined below and illustrated in Figure 1.

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- Knowledge Item: An elementary concept or skill a student can learn. These generally correspond to a specific problem type (e.g., multiplication of a pair of three digit numbers). A student demonstrates mastery of a knowledge item when they can consistently answer instances of the corresponding problem type correctly.
- Knowledge State: The span of knowledge an individual student possesses for a given subject domain. Generally defined as the set of knowledge items the student has mastered.
- Knowledge Structure: Collection of possible knowledge states that any student could achieve and dependency orders that reflect which states can be reached from others.
- Knowledge Fringe: Knowledge items that an individual student has not yet mastered, but which they are equipped to learn next based on the precedent items they have already mastered.
- Knowledge (Dependency) Map / Hasse Diagram: Analogous to a knowledge structure, except that it tracks learning dependency relations between individual knowledge items instead of between knowledge states (sets of knowledge items).

Based on the theory of knowledge spaces, our goal is to develop two general applications: (1) A dynamic assessment tool that can rapidly and precisely diagnose a student's current knowledge in organic chemistry; and (2) a personalized instruction system where problems are generated for students with individually optimized difficulty and subject material.

The first goal of a dynamic assessment system is essentially the concept of computerized adaptive testing (CAT) (*11*). While we could precisely diagnose a

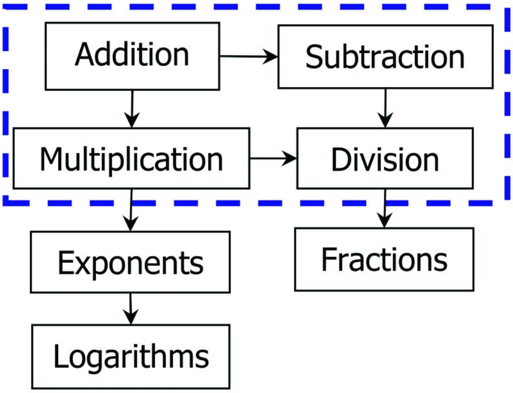

Figure 1. Simplified knowledge dependency map example applied to the subject domain of basic concepts in mathematics. The knowledge map, also known as a Hasse diagram, is a graph where each node represents a concept or knowledge item students can learn, while the arrows indicate a directed learning dependency order in the subject material. The dashed box reflects the knowledge state for an individual student, indicating that the student is competent in all of the knowledge items enclosed within the box. The knowledge items that flank the borders of the knowledge state box represent the "fringe" of the student's knowledge.

student's knowledge state by testing them on every individual knowledge item, this would be an excessive and redundant process when a student's competency in many items can be inferred from their competency in other related items. In practice, students given a CAT examination through a computer interface are first presented with a problem of "moderate" difficulty, and then, depending on whether the student answers correctly or not, the next problem is dynamically selected to be either "harder" or "easier" than the previous one. This dynamic adjustment of problem difficulty and content based on prior responses continues with each step such that the system can rapidly hone in on a precise assessment of the student's knowledge state and skill level.

The second goal of personalized instruction involves a system that delivers practice problems customized for each individual student. Assuming that the solution to the first goal successfully provides us a good diagnosis of the student's current knowledge state, we should be able to predict which problems are "too hard" or "too easy" for a student by comparing the knowledge items associated with a problem to the student's own knowledge state. With the ability to assess and predict competence, a good personalized tutorial system ought to be able to generate "useful" problems, that are situated precisely at the student's knowledge fringe.

To illustrate how a knowledge map helps one address these application goals, consider the problem of diagnosing a new student's knowledge state based on the hypothetical structure in Figure 1. A CAT examination begins by testing the student's competency in division problems. If the student demonstrates competency in division, this implies their competency in the precedent items (addition, subtraction, multiplication) and thus removes the need to explicitly test

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the student in those precedent items. Conversely, if the student is unsuccessful in the division problems, this implies that he will likely be unsuccessful in any subsequent items (i.e., fractions). Upon completing such diagnostic tests, imagine that the student's current knowledge state is represented by the items contained in the dashed box. What types of problems are "most useful" for this student to practice on? Problems based on concepts deep within his knowledge state (e.g., addition) would be "too easy" (hence boring). Conversely, problems based on concepts far outside his knowledge state (e.g., logarithms) would be "too hard" (hence discouraging), since he has not mastered the appropriate precedent concepts (e.g., exponents). The optimal problems for this student to practice on should come from the fringe of his current knowledge state, corresponding in this example to problems on exponents and fractions.

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1.2. Knowledge Spaces in Organic Chemistry

The construction of knowledge spaces and their application for assessment and personalized instruction programs has already been successful in many disciplines (*9*). Attempts to apply these concepts to the subject of organic chemistry, however, have been very limited thus far, typically, spanning only a handful of problem types and knowledge items (*12*). This limitation is related to the specific challenges posed by organic chemistry and the open-ended nature of organic chemistry problems, and has resulted in the wide usage of examinations consisting of paper and pencil problems, manually composed by human experts.

The Reaction Explorer system presents a unique opportunity to make dynamic assessment and personalized instruction a reality for the extensive breadth of content in organic chemistry. In particular, we can take advantage of over 1,500 reaction rules that have already been composed for the underlying prediction engine that drives all the reaction problems covered by the system (*13*). To do so, we simply designate each of these rules as a knowledge item in the knowledge space of organic chemistry and assess a student's knowledge of each rule based on their competency in solving problems that use the corresponding rules. By assessing the dependency relations between these rules and the typical orders in which they are learnt, we can construct a dependency diagram for the rules which will further help us to rapidly isolate a student's knowledge state, without having to explicitly test him on each one of the 1500 rules.

2. Methods

The development of dynamic assessment and personalized instruction functions for the Reaction Explorer system are primarily based on the design of 2 data structures and the implementation of 4 functional components described below and outlined in Figure 2. Important for our approach is the availability of historical data for over 2,000 students who have used Reaction Explorer at UCI over the past few years. One goal is to mine this data to organize the knowledge space.

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

Data Structures

1. Knowledge Map: Tracks the relations (dependencies and correlations) between the knowledge items (rules) used in the system.
2. User Knowledge State Model: Represents our estimate of how “competent” the student is in the use of the knowledge items (rules).

Functional Components

1. Knowledge Map Constructor: Builds the map that specifies the relations between the 1,500 rules based on a history of problem completion records by past students.
2. Knowledge Assessor: Develops a model for each student’s knowledge state based on their success / failure rate with practice problems, taking advantage of the knowledge map to infer competency of related rules.
3. Problem Success Predictor: Predicts a student’s success rate for any given problem based on the content of the problem in comparison to the model of the student’s knowledge state.
4. Directed Problem Selector: Preferentially selects problems from a batch of candidate sample problems that are optimized for each individual student in terms of difficulty and content covered.

2.1. Data Design

The basic elements in the knowledge data models described below are the over 1,500 reaction rules used by the reaction prediction expert system underlying the Reaction Explorer system. These are used in the generation, prediction, and validation of all problems in the system. We treat each rule as a knowledge item to be mastered by a student to demonstrate his organic chemistry problem-solving ability. This requires a slight variation in the interpretation of a knowledge item, in that there does not exist a one-to-one relation betweens rules and problems. In general, problems will be based on multiple rules and rules may be reused in many distinct problems. If a student answers a problem correctly, this demonstrates competency in *all* of the rules used. Conversely, if he answers incorrectly, this demonstrates a lack of competency in *at least one* of the rules.

2.2. Knowledge Map

If we treat the reaction rules used by the system as individual knowledge items in the problem domain of organic chemistry, this gives us just over 1,500 distinct items in the problem domain. The standard knowledge space structure for such a domain would consist of up to $2^{1,500}$ possible knowledge states, one for each possible subset of rules. Even with structural simplifications by culling implausible knowledge states, this is far too large a number of possible states to consider. As a result, instead of using a knowledge space structure, our knowledge map more closely resembles a Hasse diagrams that treat each knowledge item as

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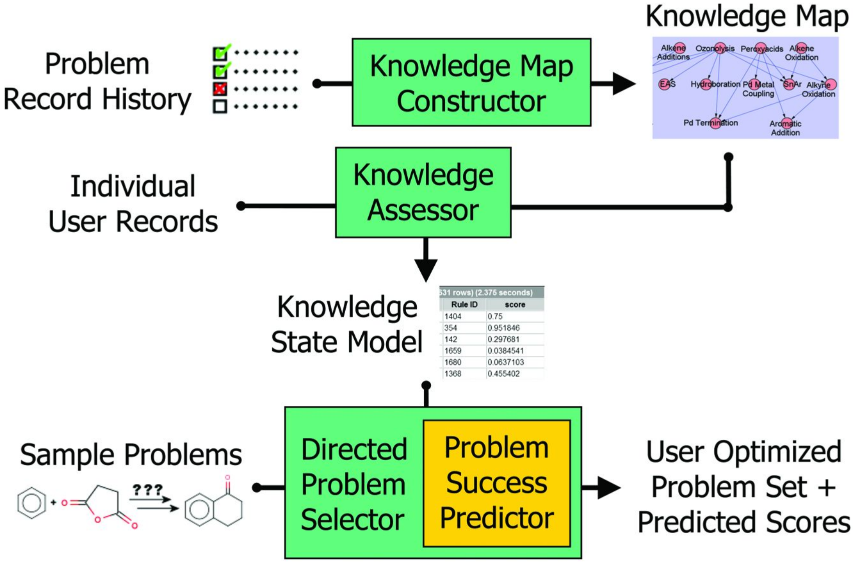
Knowledge Map
Problem Record History
Knowledge Map Constructor
Alkene Additions
Ozonolysis
Peroxyacids
Alkene Oxidation
EAS
Hydroboration
Pd Metal Coupling
SnAr
Alkyne Oxidation
Pd Termination
Aromatic Addition
Individual User Records
Knowledge Assessor
Knowledge State Model
Sample Problems
???
Directed Problem Selector
Problem Success Predictor
User Optimized Problem Set + Predicted Scores

631 rows) (2.375 seconds)

Rule ID	score
1404	0.75
354	0.951846
142	0.297681
1659	0.0384541
1680	0.0637103
1368	0.455402

Figure 2. Application functional component workflow. The knowledge map constructor performs statistical data mining on the history of completed problem records in the system to infer relations between reaction rules, thus defining a knowledge map. The knowledge assessor evaluates the record of problem attempts (successful and unsuccessful) for an individual student in combination with the rule relation information from the knowledge map to develop a knowledge state model for the student. With a model for a student's knowledge state, the problem success predictor estimates the student's probability of success for any new problem. By applying the problem success predictor to a batch of potential sample problems to deliver to the student, the directed problem selector can identify which problems would be of optimal (moderate) difficulty for the student to work on. (see color insert)

an individual node in the dependency graph, with edges in the graph representing learning dependencies.

To cope with potentially noisy data, instead of having binary edges in our knowledge map graph (either the edge exists or it does not), we use a statistical model for these dependency relationships. Specifically, we keep a fully connected graph with weighted edges between all rule pairs. In this manner, all rules are "related" to *all* other rules, but the numerical weight associated with the relation edges is graded to represent the strength of the relation.

There are actually two distinct types of rule relationships that we must track in the knowledge map. One relationship type is the "directed dependency" that has mostly been described up to this point where a user is expected to learn a rule A before they are able to learn rule B. The other relation type is a "correlation" between rules. These correlations can be due to the rules being very similar, such as the rules for "Carbocation, Hydride Shift from Tertiary" and "Carbocation, Hydride Shift from Secondary" that represent small variations on the same concept, such that it is unlikely that a user could understand one without the other.

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The other correlation possibility occurs when rules represent distinct processes, but these processes tend to always be coupled together. For example, the rule for electrophilic aromatic addition of a cation to a benzene ring will always be used in the same problem as the rule for E1 elimination back to an aromatic ring because of the necessary chain of reactivity. In this case, even though the electrophilic addition and elimination rules represent different processes, they always appear in problems together, making it unlikely that a user could demonstrate competency in one without the other.

Given the above requirements for modeling relations between rule pairs, including strong vs. weak relations and directed vs. correlated relations, our core dependency model is based on weighted relation edges between every reaction rule pair. The relation edge weighting indicates an order distance metric between the rules, modeled as a probability distribution represented by key statistics: mean, variance, and count (sample size). The particular order distance metric currently recorded is the ranking distance between when a rule A is first learned followed by when a rule B is first learned. This metric is accumulated across all students who have learned both rule A and B to produce the distribution statistics. Note that here we use the word “distance” in a loose sense, and not in its precise mathematical sense since, for instance, two distinct rules can have a distance equal to 0.

2.2.1. Order Distance Metric

To calculate the empirical order distance metric between rule pairs, for each individual student, we track when they first learned every rule and treat these as “dates of initial mastery.” The above defines a chronological learning order for every rule the student has demonstrated competency in, as illustrated in Scheme 1. The order distance between a pair of rules, A and B, is the difference in rank / position in this list between the rules. This metric can assume a negative value, indicating that rule B was actually learned before rule A. In fact, the order distance metric is anti-symmetric where the distance from A → B is the negative of B → A. Since most problems are based on multiple rules, the problem attempt date associated with all included rules will be identical, which means rules can have equal rank / position in the ordered list, corresponding to a learning order distance of 0.

2.2.2. Directed Dependency Measure

Given the order distance distribution for any pair of rules A and B, we can make qualitative interpretations of the relations between rules as described in Table 1. To develop quantitative measures, we assume the order distance metric is normally distributed across students and define a directed dependency measure for positive/forward dependencies equal to the area under the distribution curve within (0, mean), divided by the total possible area in that range (0.5). This corresponds to the ratio between the blue-shaded area in Figure 3 vs. the combined

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A → B → (C,D) → E → (F,G,H) → I → J

Scheme 1. Example of learning order for rules from which we can define an order distance metric. Rules labeled A though J are listed in chronological order by their "date of initial mastery," the date an individual student first successfully demonstrated competency in each rule. Because several rules may be included in a single problem, the "date of initial mastery" may be identical for multiple rules, resulting in the rule sets enclosed in parentheses to indicate rules mastered at the same time. In these cases, no directed learning order can be inferred for those rules. The order distance between any two rules used to define the knowledge map relations is simply the difference in rank/position in this ordering for the rules. For example, the order distance from rule A to rule E is +4 and -4 from E to A. The order distance from C to D is +2 because some rules are counted as having equal ranking (e.g., C and D).

Table 1. Qualitative interpretations of possible order distance distributions for rule pair relations

Mean	*Variance*	*Interpretation*
Large	Small	Strong Directed Dependency: When the order distance from A → B is large and positive, it suggests a directed dependency where rule B "depends on" A. That is, most students should learn A before B. Vice versa if the metric is large and negative.
Small	Large	Weak Directed Dependency: A directed dependency may exist, but the large variability in the distribution reflects a weak dependency.
Zero	Small	Strong Correlation: Implies highly correlated rules that tend to be learned near the same time.
Zero	Large	No Relation: No consistent directed dependency or correlation appears to exist between the rules at all.

area of the blue and gray-shaded sections. To measure negative/backward dependencies (where the mean value is negative), we check the area under the curve within (mean, 0) instead of (0,mean).

This method has several desirable features as a measure of directed dependency. It has possible values ranging from 0.0 to 1.0. For the directed relation from rule A to B, the value will be 0.0 if the order distance mean is non-positive and will increase towards 1.0 as the mean value increases. The distribution mean is not the only consideration however. If the variance is very large, this reflects noisy or weakly related data that should suppress the value of this measure by effectively "flattening" the distribution curve.

2.2.3. Correlation Measure

A similar measure is defined to assess the correlation between a pair of rules based on the order distance distribution. Assuming the order distance metric is normally distributed, the correlation score weight is defined as the fraction of this distribution contained within (-C,+C) where C is a correlation range parameter to be specified (currently set to 5.0). Again, this measure has desirable properties as a correlation measure with possible values ranging from 0.0 to 1.0, increasing as the order distance mean approaches 0, but being suppressed if the variance is very large.

2.2.4. Weight Scaling by Evidence Strength

A final modification to both directed dependency and correlation relation measures is to adjust their relevance based on how much evidence we have to actually believe the order distance statistics at all. In particular, the weight given to these measures is scaled down based on how much evidence we have to believe the distribution.

With no evidence (count = 0), we should give the measure a weight of 0.0. As the evidence count increases towards infinity, we should approach a full unit weight of 1.0. Many different functions satisfy these properties, including the one currently used in the system: 1 – 1/(n+1), where n is the sample size count for the probability distribution. A special exception is made if this is a "self" dependency between rule A → B when rule A is identical to B. No extra evidence is needed to have complete confidence that these are completely related, so we always give the full score weight to self-dependency cases.

2.3. User Knowledge State Model

A simple model to represent an individual student's knowledge state is a vector of competency ratings with one rating for each rule (knowledge item). To capture a richer model that can account for potentially noisy data, these are not simply binary ratings indicating "yes" or "no" for each rule competency. Instead, a numerical rating from 0.0 to 1.0 is recorded for each rule. This can be interpreted as the "expected score" or "probability of success" the user would get if presented with a problem based on the rule. To track a more detailed statistical model of each of these rule competencies, based on accumulating pieces of evidence that imply the student's competence in each rule, we again record a mean, variance, and sample size (count) to describe a probability distribution that models the student's success rate with each rule.

In a simple model, the distribution for any given student and rule is empirically based on the record of problems attempted by the student that include the rule. Every correct attempt counts as a data point with a value or "score" of 1.0 and every incorrect attempt counts as a data point with value of 0.0. In this case, the distribution mean would simply reflect the percentage of correct answers.

To enhance the model, we allow for data points that contribute less than a unit weight of relevance. This is useful when we want to develop a knowledge model while incorporating information from the knowledge map of rule relations. When a user attempts a problem that uses rule A, that not only gives us evidence for their competency in rule A, it also contributes (weaker) evidence of their competency

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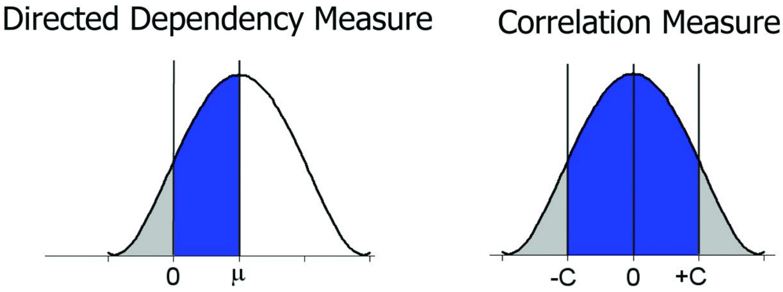

Figure 3. Visualization of quantitative measures defined for directed dependency and correlation relations based on order distance distributions. In each case, the measure is defined as the ratio of the blue-shaded area over the combined blue and gray-shaded areas. C is a correlation range parameter that must be specified externally. (see color insert)

in all rules that are “related” to A. By this interpretation, the distribution sample size statistic will no longer be an integer "count" so much as a “total weight” of evidence observed.

2.4. Knowledge Map Constructor

To construct the knowledge map described previously without manually specify relationships between 1,500 rules, we apply some simple statistical data mining to the problem completion records of over 2,000 students accumulated over the past few years of usage at UCI. For each student tracked in the system, we determine all of the rules they have demonstrated competency for, based on the problems they successfully completed, and use that to define a learning order for the rules. The idea is to find which rules the user masters over time and infer that the rules mastered at a later date are likely to "depend" on the rules mastered at earlier dates.

One caveat to beware of is that we should only attend to the “date of initial mastery” for each rule. A user may rework "old" problems with old rules much later, but this does not mean they depended on any prior knowledge. For example, consider a user who completes problems with rules in the order (1 2 3 4 5 1 2), because after they completed the problem with rule 5, they decided to go back and try rules 1 and 2 again, or maybe a later problem happened to incorporate them. This sequence suggests that rules 3, 4, 5 depend on 1, 2, not the other way around.

Once the learning order has been established for each student, the order distance between all pairs of rules covered by the student are incorporated into the respective overall order distance distribution statistics that define the relation edges in the knowledge map. Once this is repeated for all students in the records, we should have accumulated many data points of evidence for the learning order distance between every rule pair in the system.

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2.5. Knowledge Assessor

Once the knowledge map is constructed, the system can review a student's record of completed and failed problems in combination with the relation information in the knowledge map to develop a knowledge model for the student. Updating a student's knowledge model for each rule used in a problem is as simple as assigning a score of 0.0 or 1.0 to the problem (depending on whether the user successfully completed it or not) and adding that score as one more evidence data point to increment the knowledge model statistics for each rule. If one stops there however, one is only updating the knowledge model for the rules that were explicitly tested.

To infer more information about a student's knowledge model, the system performs a second-order update on the model for all rules that are "related" to the ones actually used in a problem. First, the correlation measure between the rules used in the problem and all other rules is calculated and the student's knowledge statistics for all of these correlated rules is incremented with another data point with value equal to the problem score (0.0 or 1.0). However, this new data on correlated rules is not given a full unit weight count of 1. Instead, this second-order data is weighted based on the correlation measure, indicating the strength of correlation between the second-order rules and the ones actually used in the problem. This process is repeated similarly for directed dependency relations between the rules, with second-order data points weighted by the directed dependency measure between the rules in the problem and all other second-order rules. In the directed dependency case, one must make an additional modification depending on whether the problem was successfully completed or not. If the problem was successfully completed, then we *increase* the score statistics for all second-order rules that come *before* the problem's rules in the directed learning order. Conversely, if the problem was not completed successfully, then we *decrease* the score statistics for all second-order rules that come *after* the problem's rules in the directed learning order.

For students that are new to the system, where no prior information is available on their competence in any rule, a default uniform prior estimate score of 0.5 is assigned for all rules with an evidence weight count of 1. As the user attempts problems in the system, this will contribute actual evidence to the knowledge model which will rapidly diminish the relevance of this prior estimate. As the evidence accumulates for the knowledge model of any rule, a cap is imposed on the effective evidence count used to calculate the statistics (10 in the current system) which has the effect of giving greater weight to the most recent evidence data points. This is important for addressing the issue that a user's knowledge state is not a static entity, but should evolve over time. Thus, even if a student gets a rule incorrect 100 times in a row, if they subsequently get it correct 10 times in a row, we should have a strong belief in their current knowledge of that rule based on the recent evidence, rather than aggregating the entire history and assuming the user only has a 10% chance of correctly using the rule. Another implication of the evolving knowledge state is that these updates to a user's knowledge model should be done in "real-time," immediately after a user attempts a problem, as

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opposed to the knowledge map construction which can be managed as a periodic batch process.

2.6. Problem Success Predictor

With the ability to model a student's knowledge state and assess problem difficulty and topic coverage, the key function that would empower essentially all desirable features of this system is the ability to predict a student's problem solving ability. In particular, given any arbitrary problem and student, predict the expected score or the likelihood that the student will correctly answer the problem. This prediction is based on which rules are used in the problem and our knowledge model estimates for the user's competence in each rule. The current approach is simply to take the student's mean success rate score for each rule used in the problem and combine these into an aggregate score. To aggregate the scores, currently we use the minimum or "worst" predicted score amongst all rules used based on the idea of a "weakest link" in the problem. That is, a student's ability to successfully complete a problem is limited by whichever rule the student is worst at.

2.7. Directed Problem Selector

Once the entire knowledge map is constructed and a student's current knowledge state is modeled, the ultimate desirable feature is to deliver a personalized learning experience. In particular, problems generated for the student should be adapted to the optimal subject material and difficulty. The problem success predictor provides the core function needed to deliver these personalized problems. In general, all we must do is preferentially generate and select problems for the student where the predicted probability of success is as close to 50% as possible. If it were close to 100% (problem is too easy) or 0% (problem is too hard), there is not much point in testing them since the outcome is essentially a foregone conclusion and neither we nor the student will learn much from their problem attempt. Problems with near 50% probability of success represent the "most useful" practice problems based on material that the student has some understanding of, but needs further practice to master.

A slight distinction should be made between diagnostic vs. practice problems. Conceptually, a student should first be given diagnostic problems based on material that we have little data to estimate their competency in. After the results of these diagnostic problems inform our model of the student's knowledge state, we can then deliver appropriate practice problems with estimated success near 50%. In actual usage, all problems have some diagnostic value, so we need not make a sharp distinction between these problem types. In particular, by setting the default prior estimate for knowledge success rates to 0.5, preferentially selecting problems with estimated success near 50% will naturally pick up both good diagnostic problems and good practice problems. Once the student has completed a battery of problems, "good diagnostic problems" will not really be needed since a knowledge model will already have been developed for the student with success estimates for all rules in the system (even if the estimates are based on second-order inferences).

3. Results

Using the methods described above, a knowledge map for organic chemistry has been constructed for the Reaction Explorer system based on 123,903 problem completion records of 2,152 distinct users and is periodically updated as more users complete problems in the system.

Figures 4a and 4b provide a simplified visualization of the current knowledge map, with rules aggregated into subject topics corresponding to chapter sections of an organic chemistry textbook (*14*). Though some correlation can be observed, it is clear that the aggregate learning order of students who have used the system do not closely follow the chapter order of this textbook. This is not surprising as the course plans followed by the students who have used this system have varied across several textbooks (*15*, *16*) and subject orders (e.g., some of the courses have taught carbonyl chemistry before aromatic chemistry, despite aromatic chemistry coming first in the textbook's chapter order).

An interesting finding in the knowledge map construction is that, of the over 1,500 rules included in the system, only 629 are ever actually used to successfully solve problems and become part of the knowledge map. This can be explained in part because some rules are designed to catch problematic reactions that would never be used in a successful synthetic reaction (e.g., neutralization of an organometallic reagent in protic solvent). Since the knowledge map only concerns itself with rules that are useful for successfully solving problems, these "error catching" or "warning" rules do not apply in the knowledge map. The other major explanation is that many of the rules are similar enough to the point of redundancy, thus some are never invoked when alternative forms are available to use first.

With the knowledge map in place, the system updates a model of each student's knowledge state in real-time as they attempt problems. This allows the system to dynamically predict a student's probability of success for any given problem. System usage is still largely based on students requesting "random" problems to work on, but the system now exploits the student's knowledge model to deliver a more directed experience. In particular, when a user requests a new problem to work on, the system will actually produce a battery of many candidate problems that satisfy their request. The system predicts the user's probability of success for each of these problems and then preferentially selects one for the user with predicted probability of success close to 50%.

4. Discussion

The Reaction Explorer tutorial system for organic chemistry, which already delivered a uniquely flexible and rich learning experience based on an underlying predictive model of chemical reactions, has been upgraded to support dynamic assessment and personalized instruction functions based on concepts from the

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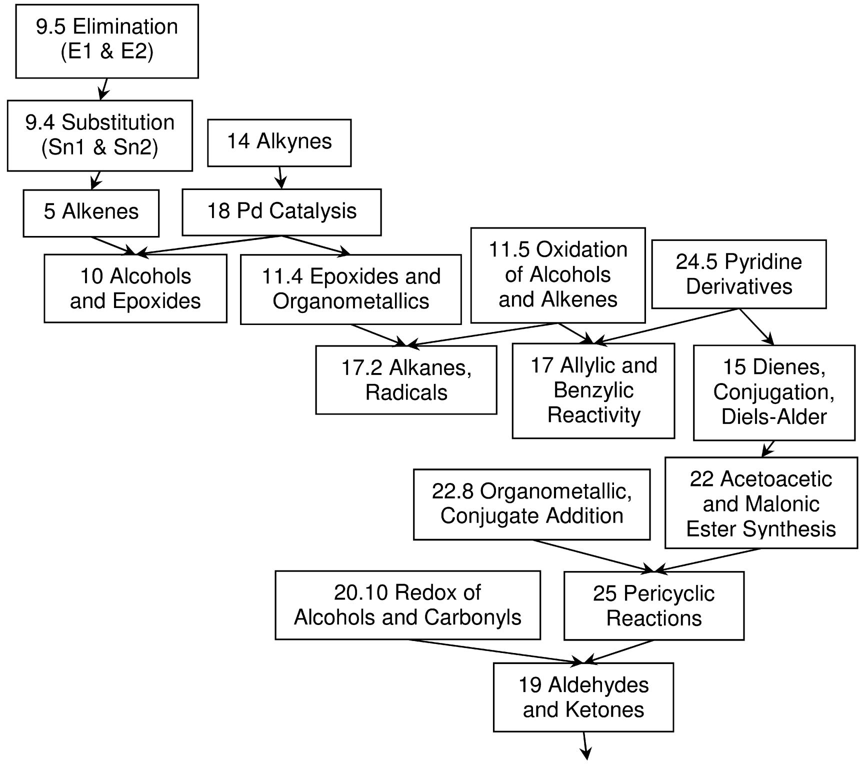
9.5 Elimination (E1 & E2)
9.4 Substitution (Sn1 & Sn2)
14 Alkynes
5 Alkenes
18 Pd Catalysis
10 Alcohols and Epoxides
11.4 Epoxides and Organometallics
11.5 Oxidation of Alcohols and Alkenes
24.5 Pyridine Derivatives
17.2 Alkanes, Radicals
17 Allylic and Benzylic Reactivity
15 Dienes, Conjugation, Diels-Alder
22.8 Organometallic, Conjugate Addition
22 Acetoacetic and Malonic Ester Synthesis
20.10 Redox of Alcohols and Carbonyls
25 Pericyclic Reactions
19 Aldehydes and Ketones

Figure 4a. Simplified dependency diagram derived from the system's current knowledge map for organic chemistry. This diagram is provided as a convenient visualization, but the actual knowledge map used by the system consists of a fully connected graph of weighted relation edges connecting hundreds of nodes representing knowledge item rules. To produce the simplified diagram, rules are aggregated into subject topics corresponding to numbered chapter sections of an organic chemistry textbook.

theory of knowledge spaces. By performing statistical data mining on a history of problem completion records, a knowledge map is constructed for the system to specify the correlations and directed learning dependency orders for the reaction rules that drive the problems generated by the system. This knowledge map enables support for dynamic assessment where the system can rapidly and precisely model a user's knowledge state based on their record of problem attempts. This assessment includes estimation of the user's competence in each of the underlying rules used in the problems, while taking advantage of relation information in the knowledge map to infer competency in all subjects without having to actually test the user on every single rule. Finally, models of individual user knowledge states allow the system to predict each user's probability of success for any given problem, which in turn allows the system to optimize learning trajectories by preferentially selecting user practice problems that are neither "too hard" nor "too easy" for the individual user.

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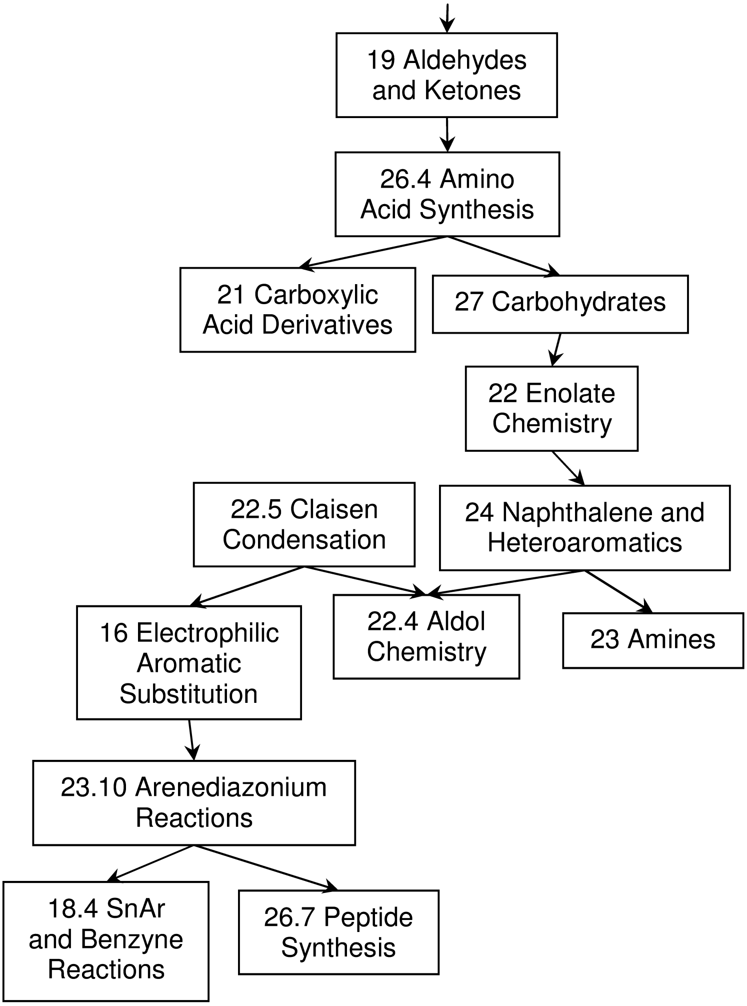
19 Aldehydes and Ketones
26.4 Amino Acid Synthesis
21 Carboxylic Acid Derivatives
27 Carbohydrates
22 Enolate Chemistry
22.5 Claisen Condensation
24 Naphthalene and Heteroaromatics
16 Electrophilic Aromatic Substitution
22.4 Aldol Chemistry
23 Amines
23.10 Arenediazonium Reactions
18.4 SnAr and Benzyne Reactions
26.7 Peptide Synthesis

Figure 4b. Second half of the simplified visualization for the current organic chemistry knowledge map. After aggregation of rules into subject topics, the weight of relations between subject topics was calculated as the average relation value for all rule pairs that span the topic pairs. The relation edges between topics were then pruned down to a minimum spanning tree. Tree layout is organized such that all remaining directed edges point downwards and do not traverse more than a single row of topics.

Work is ongoing to validate the methods and results described here as well as explore alternative models. The key module for testing is the problem success predictor. Validating that this module reliably predicts the probability of success for any given student and problem provides a basis for confidence in all of the knowledge modeling processes up to that point and in the problem selection processes thereafter. A validation process currently ongoing is to train the system's knowledge state model for any given user, but only including problem records up to fixed date, and then testing whether the system can reliably predict the user's success in the problem records after that date.

Many details of the system described in this Chapter are somewhat ad hoc and a more principled approach is currently under investigation. Furthermore, the system described here includes several parameters and definitions that are open to interpretation and optimization. For example:

- Correlation measure range parameter: The correlation measure between rule pairs is currently defined as the fraction of the order distance distribution for each rule pair that is within (-C,+C) where C is a range parameter that must be specified.
- Problem "expiration" period: Once a user begins a problem attempt, if they do not successfully solve the problem within this time, it will be counted as incomplete in terms of developing their knowledge model. Current setting is 5 minutes, which covers just over 85% of the history of completed problems.
- Default prior knowledge score and weight: For new users, when no prior information is implied regarding their knowledge state, the default success rate assigned for any rule is 0.5 with an evidence weight count of 1.
- Date of initial mastery: For developing the knowledge map and defining learning orders, the system credits a user with being competent in the use of a rule as soon as they successfully complete a single problem that includes that rule. This is not a very robust definition due to the possibility of "lucky guesses" or users forgetting previously learned material, though it is very helpful as a simplifying assumption to streamline the knowledge mapping process.
- Problem difficulty: As estimated by the problem success predictor, difficulty is simply based on the success rate estimate for the "worst" rule used in a problem. This accounts for the knowledge necessary to solve the problem, but arguably there is a distinction between the *knowledge* needed to solve a problem based on recall of facts vs. the "*skill*" needed to solve large, multi-step problems that incorporate many facts.
- Useful problems: For a given user, in this Chapter we have proposed to select problems where the user has an estimated 0.5 probability of successful completion. It may be that problems with a higher probability of completion (e.g. 0.75) may be more suitable and provide a better learning experience.

All of the parameters and definitions above should be adjusted to optimize system accuracy and user learning performance. This parameter optimization process is a natural follow up project, though it must wait until the automated validation method is in place so that the results of different parameter and definition combinations can actually be compared against each other to identify superior settings.

The above still only refers to validation of the system's problem success prediction capabilities, but ultimately the actual outcome measure students

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and instructors are interested in is whether use of the system's new features actually impact student knowledge as measured by external examination scores. Classroom trials similar to the ones previously completed to assess the core functions of Reaction Explorer (*7*) are necessary to assess such an outcome measure. Such a study is always vulnerable to criticism regarding bias in participant self-selection, variability in instruction and examination, etc. One feature we can take advantage to differentiate the core Reaction Explorer functionality vs. the core functions *plus* personalized instruction is that the personalized instruction features largely happen behind-the-scenes beyond the perception of the student user. The relative transparency of the personalized instruction features makes it relatively easy to assign users to cohorts in a random and blind manner. For example, any user whose student ID number ends with an even number could be assigned to the core function group where the system will not try to preferentially select problems of "moderate" difficulty and will instead just deliver uniformly "random" problems just as it has before, while users whose student ID number ends with an odd number would be given problems based on the personalized instruction functions.

While various optimizations and validation experiments must be completed to increase confidence in the intended effects of the new knowledge map based functions of the Reaction Explorer system, the methods described above and implemented in the system have already laid the groundwork and infrastructure to make dynamic assessment and personalized instruction possible for the complex subject domain of reactions in organic chemistry.

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Chapter 12

Site Under Construction: Designing a Successful Online Course

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This chapter discusses important pedagogical and technical aspects for developing a successful online course, and it describes how each of these aspects influenced the development of an online course about nanoscience aimed at teachers. In order to maximize learning in the online setting, the course developer must consider many things including the content, the course layout, avenues for communication, and how to moderate the interactions of all participants. Of significant importance is to ensure a high degree of interactivity in the online environment. Three types of participant interactivity should be considered: interactivity with the content, with the instructor, and with peers. An understanding of the impacts of each of these aspects will help the course developer design a virtual classroom that maximizes the learning of all course participants.

Introduction

Designing an online course can seem like a daunting task if one is not already familiar with the process and with current pedagogical techniques for creating a successful online learning environment. Over the past decade, there has been an explosion of interest by universities and colleges for developing online classes as a means for increasing student enrollment and revenues, and for reaching non-traditional students and wider audiences. In some cases, the

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

issue of online teaching and virtual universities has become politicized (*1*). For example, as discussed by Coppola et al., Faculty at the University of Hawaii have gone on strike to protect their intellectual property rights of material created for online courses (*1*). Some faculty at the University of Washington opposed their governor's push for creating virtual universities in place of building physical campuses by signing an open letter. Opponents to online learning fear there is an impersonal automatic nature to the process, or that we are creating "digital diploma mills" (*2*). Some have argued that online courses lack the intellectual integrity and rigor that face-to-face courses have. However, numerous studies have refuted this argument, showing that just as in traditional classrooms, when the appropriate goals are set, high quality learning occurs in online courses. There is now a drive to ensure that online courses and programs provide high quality learning opportunities that are either as good as or sometimes better than those in a face-to-face class.

In this chapter, we discuss those design features and pedagogical aspects that helped us create a successful online course about nanoscience for teachers, called "Nanoscience for Teachers". We developed the course as part of the Nanoscale Science and Engineering Center at the University of Wisconsin-Madison beginning in 2004 (*3*, *4*). In the early 2000s, the topic of nanoscience began to reach more mainstream audiences, with increasing news stories about possible technical, medical, and environmental advances nanotechnology might bring society. At the time, NSF predicted nanotechnology would form a trillion dollar industry by the year 2015 (*5*). Along with this explosion of interest in nanoscience came a drive to incorporate it into educational curricula at all levels (*6*). In order to reach a generation of students, it was necessary to provide continuing education opportunities for their teachers. One convenient way of reaching an audience of teachers from across the country is through an online course.

Since its first offering in the summer of 2006, the course has had multiple iterations and reached an estimated 40 teachers from across the country (and in some cases the world). Teachers taking the course have gained a broad background in the subject of nanoscience and prepared nanoscience teaching modules to use with their own students. In addition to imparting knowledge to teachers, the course has been successful at creating a community of learners who have indicated the course was a very positive and helpful experience for them (*7*).

This chapter will take the reader through the process of creating Nanoscience for Teachers, from the initial stages of choosing course content and arranging course layout, to the methods used for ensuring high levels of interactivity in the online environment. Along with the description of our own online course, we summarize relevant literature findings and their influence for course design throughout this chapter. The topics we discuss here have broad-reaching applications no matter what the subject of the online course you may be building. Table I summarizes the important aspects that will be discussed.

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Table I. Chapter Outline

Online Course Design:

Choosing Content

- *Accuracy and Relevance of Content*
- *Laboratory and Hands-On Experience*
- *Finding Reliable, Stable Web Content*
- *Copyright Considerations*
- *Content Layout and Course Management Systems*

Interactivity

- *Interactivity with Instructor*
- *Interactivity with Peers*
- *Interactivity with Content*

Conclusions

Online Course Design

Choosing Content

Ensuring your online course has appropriate and useful content is a crucial component for creating a successful learning environment. Many of the same basic principles governing course content apply in the virtual classroom just as they do in a face-to-face course. The instructor must provide students with meaningful subject matter that is connected to previous knowledge and relevant to students' lives. The course content must be at an appropriate level relative to the background knowledge students bring to the course. The quantity of content must be appropriate to achieve course goals and not so great that students will not be able to assimilate and digest it within the time frame of the course. Finally, the content must be capable of being delivered online; this can be a problem when hands-on work by the students is important. In this section, we discuss the process for choosing the content for Nanoscience for Teachers, as well as copyright issues one should be aware of when building the online course.

Before we even began developing the online course, we had to first assess whether or not there was enough material about nanoscience specifically geared towards a general audience. When this work began in 2004, discussions about the importance for educating the public about nano were just beginning in the field. Many felt that society (especially the next generation of students) needed to be educated about the field in order for it to reach its full potential (*5*, *6*, *8*).

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Table II. Topics in Nanoscience for Teachers, Chosen Based on Interviews with Content Experts

Topic #	***Topic Title**: Description*
1	**Introduction to Nanoscience**: Basic ideas and potentials of the field
2	**The Nanoscale**: How small is the nanoscale? How can we understand of the size if we cannot see it?
3	**Properties of Nanomaterials**: Special characteristics of materials at the nanoscale
4	**Measuring Nanoscale Structures**: Instruments used by nanoscientists (AFM, STM, etc)
5	**Synthesis of Nanomaterials**: Top down and bottom up approaches
6	**Health and Environmental Effects**: Advances and potential hazards nanotechnology may bring
7	**Nanotechnology and Medicine**: Potential advancements nano may bring to the field of medicine
8	**Nanotechnology in Nature**: Nature is the first nanotechnologist; example nanomachines such as motor proteins
9	**Societal Implications of Nanoscience and Nanotechnology**: What should we, as educators, make sure our students understand about nanoscience so that we have an educated society that can make informed decisions for legislation?

Accuracy and Relevance of Content

We began the intensive process for choosing course content by interviewing three nanoscience researchers who are also faculty at a major research university. We asked them questions such as, “What are the most important aspects about nanoscience you want your students to know?”, “Are there any general nanoscience textbooks that you would recommend?” We felt it was important to choose content relevant for our audience of teachers, who would be concerned primarily with learning the material to take back to their own classrooms. Therefore, ideally we looked for content that was for a general audience of teachers with some background in science (chemistry, or physics), but little or no background in nanoscience. From our interviews with researchers and nanoscience educators, we condensed a list of nine important nanoscience topics to cover in our course (See Table II).

In our particular situation, we felt that it would be beneficial to have a required textbook. Other situations may not necessitate a textbook, depending whether all the material could be presented through the online course. One advantage of having a textbook is that it supplements the online content. In our case, it unified the central theme of the course and provided general knowledge to aid in understanding more specific articles we included online. The textbook readings also served as a basis for online class discussions through forums and email (as discussed below). At the time, most textbooks on nanoscience were geared to a highly specialized audience, and were not appropriate for our continuing education course. We were able to find one for a very general audience (*9*). In subsequent offerings of Nanoscience for Teachers, we added a second book geared specifically towards educators and containing suggested activities to use with students (*10*). Participants could order these textbooks online through Amazon.com.

Laboratory and Hands-On Experience

As many chemical educators know, a crucial aspect for learning chemistry is gaining hands-on experience in the laboratory. It can certainly be difficult to include hands-on content in the virtual classroom. One early example for providing at-home students with applied lab experience was the work by Kennepohl (*11*). In his study, distance learning students were given home-study microlab kits, containing the laboratory supplies and instructions for completing the experiments at home. Whenever possible, students used reagents commonly found in the home, such as coffee grounds and corn syrup (*11*). Others have incorporated virtual laboratories into their online courses (See for example Elliot and Kukula (*12*)). Some common methods for delivering a virtual laboratory include LabVIEW, Virtual Network Computing, CD-ROM, or online sites that have laboratory simulations or videos, such as the ChemCollective Virtual Laboratory (*13*), Late Nite Labs (*14*) or YouTube.

The University of Wisconsin-Madison MRSEC Interdisciplinary Education Group has created a Virtual Lab Manual that is ideal for educators (*15*). This Virtual Lab Manual has a variety of laboratories related to nanoscience and materials science that range in difficulty from middle school, to high school, and to college level. In Nanoscience for Teachers, we linked to at least one of these virtual laboratories per topic, so participants could see suggested labs they could do with students on a particular nanoscience subject.

We also felt that the course content should have a unifying purpose, relevant to our teachers' profession. Therefore, we had our participants compose a nanoscience teaching module as a final project. Teachers could use any of the content provided through the online course to develop a unit plan or nanoscience-related activity they could share with their students. To help increase peer interactivity in the course (as will be discussed further below), we had our teachers upload their modules to the course and then peer review the projects. As a result, our participants gained something useful for their classrooms, which encouraged the teachers to pass along their newfound knowledge to their students (*3*, *7*).

Finding Reliable, Stable Web Content

Generally speaking, we searched for content for our online course that was available on the Web on reliable and stable Web sites. Finding online resources was made easier through online search engines such as Google.com. Finding quality

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resources online could be challenging at times; we found that certain science news sites were the most reliable and provided most accurate information. For example, Physorg.com had focused articles related to our weekly topics, so we searched it (and other similar) sites directly. We then incorporated direct links to these articles and sites into our course. When performing Internet searches, we suggest you begin by using a search engine to find sites broadly related to your topic. Evaluate the sites with regard to quality of scientific information and whether the site is likely to be available in the long term. We then suggest you search within those reputable sites for more specific material related to your topic. Your choice of resources to include in the online course may depend on whether or not they are copyrighted, as discussed in the next section.

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Copyright Considerations

You might be familiar with the recent intense battle by the music and entertainment industries to crack down on copyright violators who illegally download intellectual property. Never before in our history has it been so easy (with the click of a button) to obtain copies of material and then to replicate and distribute it. It is not appropriate to use someone else's creative material without either attribution or permission and it is also illegal, with severe penalties for copyright infringement. It is of utmost importance that course developers are knowledgeable of copyright laws; they should seek counsel from, and work with their university's library and legal personnel in order to ensure that the material used for the online course is obtained and presented in the course legally. One should consult the Digital Millennium Copyright Act (DMCA) (*16*) and the Technology, Education, and Copyright Harmonization Act (TEACH Act) (*17*) for laws on the way educators can use copyrighted material in the online course (for an overview see the slideshow by Renee Hobbs based on her book, Copyright Clarity: How Fair Use Supports Digital Learning) (*18*).

An easy to understand online slideshow about redistributing online content and intellectual property rights is the one by Creative Commons (*19*). This describes the four types of creative commons licensing commonly used online: 1) Attribution—lets others freely redistribute materials as long as attribution to the original creator is given; 2) Noncommercial—others may redistribute the material with attribution, but cannot profit from use of the material without the author's permission. Users must also provide a link to the license so others know how to use the media; 3) No Derivative Works—lets others redistribute the media, but only without changing it; 4) Share Alike—lets others build and change the media, but they must make the resulting media available to others on the same terms as the original piece.

See the recent article by Johnson for an example of the protocol for intellectual property in distance education at one university (*20*). In this protocol, the university prefers that course developers create their own original content for the online course. In this case, the developer should understand the university's policy on intellectual property rights for any original material created by the developer. Different universities have different policies; some universities maintain the rights to all materials created by the developer, while others allow the developer to retain some or all rights (*21*).

As Johnson explains, if the developer wants to use an external intellectual property, the university must obtain permission from the copyright holder to use it in the online course (*20*). If the external intellectual property is in the public domain, no further effort is necessary and the developer can use the piece in the course; however, it can be difficult to determine whether a resource is in the public domain, so the developer should seek assistance in verifying this. Ideally, the developer can place a link in the course to the external resource if it is in the public domain and available on a reliable and stable Web site. This is more desirable than downloading and copying the resource and placing it in the course. If a material is not in the public domain, the university library might have a subscription or be able to obtain permission to access the material. In this situation, the material is made available through the university's course reserve system, which can be accessed through a link in the course that connects participants to the library's online reserve system.

In Nanoscience for Teachers, most of the content is linked to external sources that are in the public domain and available on reliable and stable Web sites. From year to year the links must be updated and fixed if they become broken. Many of the excellent nanoscience educational resources linked to are from the University of Wisconsin-Madison Materials Science Research and Engineering Interdisciplinary Education Group (*15*) and the Nanosense Group of SRI International (*22*). In the next section we discuss key points for arranging the content once it has been chosen for the online course.

Content Layout and Course Management Systems

After deciding on course content, the developer must next consider how to arrange the content in an online space. Research has shown that an online course should have a clear structure and straightforward layout to maximize student learning (*23*). Unless one has a very strong background in Web design, it is helpful to use an online course management system (CMS). With a CMS, the course developer no longer needs to use HTML or other markup languages to build an online course from scratch. The CMS is a ready-made program that does the HTML programming for the user helping to create and arrange the content. The CMS houses the online course and organizes the content in a straightforward and ordered manner. Readers might already be familiar with one or more of the common Web course management programs: Blackboard Learning System (*24*), Desire2Learn (*25*), SharepointLMS (*26*), and Moodle (*27*) are some examples.

The online course management system known as Moodle permitted us to have a large degree of control over how we arranged the course content in Nanoscience for Teachers (*27*). Moodle was developed based on constructivist pedagogies, and its features allow for high degrees of interactivity in the course (*28*). Further, Moodle is a free, open-source system that has a thriving support network of experienced users. Instructions for installing Moodle on a server are relatively easy to follow, and a course developer has the maximum amount

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of control over the course when he or she sets up the server by him or herself. Many institutions of higher education are experimenting with Moodle because of its open-source aspect, so scout around to see whether Moodle is available and supported by your institution before deciding to use one of the for-profit systems mentioned earlier. Having support from campus information technology staff is not essential, but often useful.

Here are some of the standard features in Moodle. Users can participate in forum discussions and online chats, complete quizzes, submit written assignments, complete group projects, write in journals, use the wiki tool to develop a course glossary or other course material that all participants can edit, search forums for specific comments, and send emails to individual users or the whole class. Additionally, the course instructor can choose to grade any of the aforementioned student tasks, and organize the course grades using the gradebook. Because Moodle is open source, other users are constantly programming add-on features into Moodle that they can make available for anyone to download and add to their own course. For example, Moodle experts at the University of Wisconsin-Madison have created add-ons to allow students to make drawings (including molecular structures) in answers to questions, to facilitate entering mathematical expressions in answers to questions, and to enable individualized feedback in response to student answers for essay-type quiz questions. Other users have developed hundreds of add-ons, such as those for incorporating Web conferences, converting text-to-speech, or connecting Moodle to Facebook.

In Nanoscience for Teachers, we used the standard installation with a few add-ons to organize the course. When participants login to the course, they come to the homepage (Figure 1), which organizes the nanoscience content down the center of the page. In this section, links to course pages and external resources are provided; each link is clearly labeled so the user will understand where the link leads. To the right and left of the content section of the screen, there are within-course links that take the user to various assignments (quizzes and workshops) and user forums. A summary of the features we incorporated is in Table III. These are what we chose for Nanoscience for Teachers, but many other features might be suitable for other courses.

As one might imagine, there is much more to developing a successful online course than just choosing and arranging content. In the next section, we discuss a crucial aspect for creating a community of learners online: ensuring high levels of interactivity in an online course.

Interactivity

One of the most important characteristics for any online course is its level of interactivity. There has been much research in the literature on increasing interactivity in a computer mediated classroom (see for example Swan, 2001 (*29*) and references therein). Three kinds of interactivity can be defined in an online course: interaction with content, interaction with the instructor, and interaction with peers (*30*). The influence of each type on student learning and satisfaction has been investigated, as well as the relationship among these three types of interactivity.

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Table III. Nanoscience for Teachers Course Features and Descriptions

Course Feature	*Description*
Announcements	Posted weekly or daily in a forum; also sent out to users via email
Assignments	Participants upload papers describing their current curricula
Forums	Participants post comments and discussion items here; all posts are also sent to users via email
Quizzes	Essay-type questions; untimed; participants can save and resume quizzes later; Quizzes are posted at the beginning of the week; participants take the quiz after completing the assigned readings for that week
Resources	Links to all the various external sources; also accessed in the center of the page under each topic.
Surveys	A collection of built-in surveys for assessing the learning environment in the course (*3*, *28*).
Workshops	Allows group-work and peer-reviewing of projects; used in this research as a means for providing anonymous peer feedback for individual final projects
Chats	Synchronous discussions with all users logged in simultaneously

Interactivity with the Instructor

The role the instructor plays in an online learning environment is very important, just as it is in face-to-face courses. Researchers have found that students in an online course experience more meaningful learning when the teacher is highly involved in the course and serves to model discourse among the participants (*31*).

Instructors in either a traditional or virtual classroom have been described as having three main roles: cognitive, affective, and managerial (*1*). The cognitive role includes direct instruction, and the affective role includes aiding course communications through verbal behaviors and through non-verbal expressions or gestures. The managerial role includes tasks such as course design, administration, and student supervision.

Coppola, Hiltz, and Rotter have studied the ways these instructor roles change in the online setting (*1*). The researchers interviewed faculty teaching online courses in online undergraduate and graduate programs. For some of those interviewed it was their first time teaching an online course. Regarding changes to the cognitive role, the faculty indicated that in the online setting there was more time to reflect on a student's question before answering. They also reported that learning became more of a two-directional process, with the instructors learning from their students and vice versa. They also found that teachers used the Socratic method more online by guiding student learning through back-and-forth questioning.

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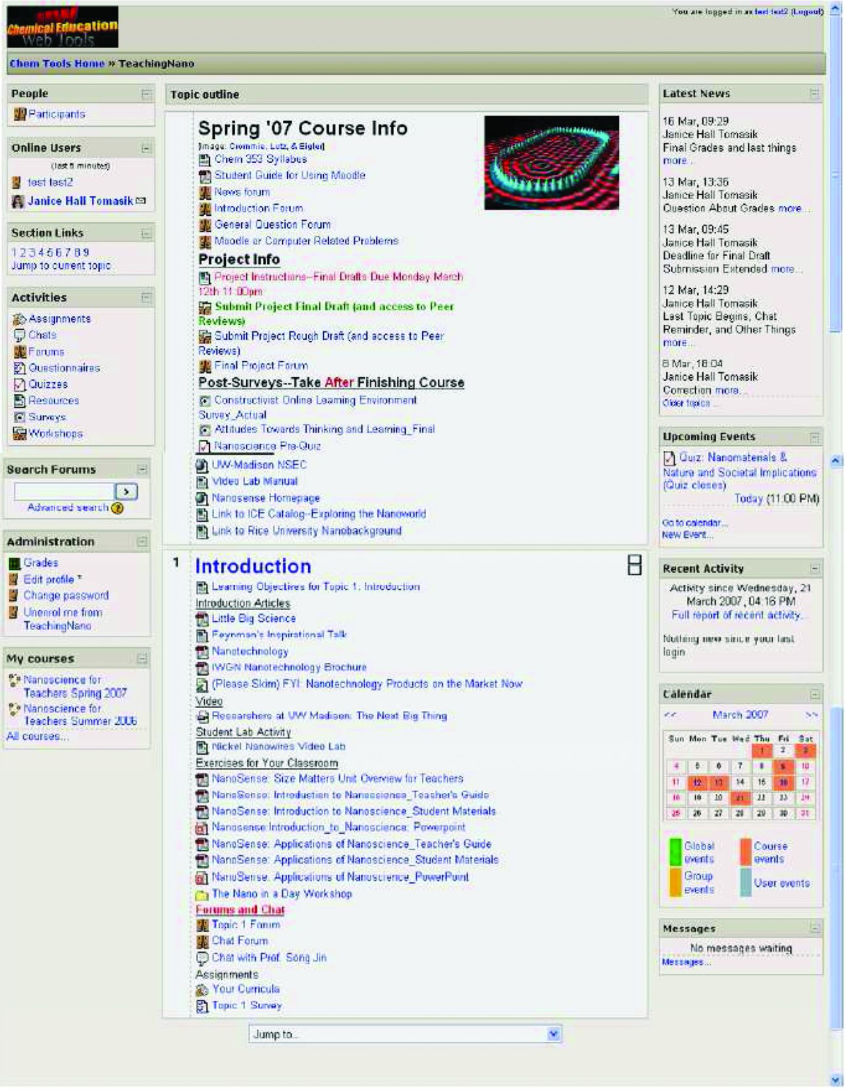
Chemical Education Web Tools
You are logged in as test test2 (Logout)
Chem Tools Home » TeachingNano
People
Participants
Online Users
(last 5 minutes)
test test2
Janice Hall Tomasik
Section Links
1 2 3 4 5 6 7 8 9
Jump to current topic
Activities
Assignments
Chats
Forums
Questionnaires
Quizzes
Resources
Surveys
Workshops
Search Forums
Advanced search
Administration
Grades
Edit profile *
Change password
Unenrol me from TeachingNano
My courses
Nanoscience for Teachers Spring 2007
Nanoscience for Teachers Summer 2006
All courses...
Topic outline
Jump to...

Spring '07 Course Info

[Image: Crommie, Lutz, & Eigler]

Chem 353 Syllabus
Student Guide for Using Moodle
News forum
Introduction Forum
General Question Forum
Moodle or Computer Related Problems

Project Info

Project Instructions--Final Drafts Due Monday March 12th 11:00pm
Submit Project Final Draft (and access to Peer Reviews)
Submit Project Rough Draft (and access to Peer Reviews)
Final Project Forum

Post-Surveys--Take After Finishing Course

Constructivist Online Learning Environment Survey_Actual
Attitudes Towards Thinking and Learning_Final
Nanoscience Pre-Quiz
UW-Madison NSEC
Video Lab Manual
Nanosense Homepage
Link to ICE Catalog--Exploring the Nanoworld
Link to Rice University Nanobackground

1 Introduction

Learning Objectives for Topic 1: Introduction

Introduction Articles
Little Big Science
Feynman's Inspirational Talk
Nanotechnology
IWGN Nanotechnology Brochure
(Please Skim) FYI: Nanotechnology Products on the Market Now

Video
Researchers at UW Madison: The Next Big Thing

Student Lab Activity
Nickel Nanowires Video Lab

Exercises for Your Classroom
NanoSense: Size Matters Unit Overview for Teachers
NanoSense: Introduction to Nanoscience_Teacher's Guide
NanoSense: Introduction to Nanoscience_Student Materials
Nanosense:Introduction_to_Nanoscience: Powerpoint
NanoSense: Applications of Nanoscience_Teacher's Guide
NanoSense: Applications of Nanoscience_Student Materials
NanoSense: Applications of Nanoscience_PowerPoint
The Nano in a Day Workshop

Forums and Chat
Topic 1 Forum
Chat Forum
Chat with Prof. Song Jin

Assignments
Your Curricula
Topic 1 Survey

Latest News

16 Mar, 09:29
Janice Hall Tomasik
Final Grades and last things more...

13 Mar, 13:36
Janice Hall Tomasik
Question About Grades more...

13 Mar, 09:45
Janice Hall Tomasik
Deadline for Final Draft Submission Extended more...

12 Mar, 14:29
Janice Hall Tomasik
Last Topic Begins, Chat Reminder, and Other Things more...

8 Mar, 16:04
Janice Hall Tomasik
Correction more...
Older topics...

Upcoming Events

Quiz: Nanomaterials & Nature and Societal Implications (Quiz closes)
Today (11:00 PM)
Go to calendar...
New Event...

Recent Activity

Activity since Wednesday, 21 March 2007, 04:16 PM
Full report of recent activity...
Nothing new since your last login

Calendar

<< March 2007 >>

Sun	Mon	Tue	Wed	Thu	Fri	Sat
				1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31

🟩 Global events
🟥 Course events
🟧 Group events
🟦 User events

Messages

No messages waiting
Messages...

Figure 1. Screenshot of Nanoscience for Teachers, Spring 2007

The affective role online also differed from the face-to-face environment. In a traditional classroom, the instructor uses a variety of verbal and non-verbal cues for communication that can lead to increased learning (*32*). In the virtual setting non-verbal communication techniques, such as eye contact and physical gestures are not possible. Instructors and students must find other means for conveying these signals to each other. Researchers have found that online course participants project their personal identities and emotions through verbal "immediacy" behaviors alone (*33*). Immediacy behaviors refers to those communications that enhance closeness to others and decrease social distance (*34*). Online participants have adapted to portray emotions and non-verbal expressions by using emoticons (such as ☺), humor, and self-disclosure (*33*, *35*, *36*).

Indeed, the faculty in the study by Coppola et al. did note the lack of physical avenues for communication (*1*). In one case, the instructor needed to clear up confusion with some course participants over the phone. However, in spite of this lack of a physical environment, the instructors believed their communication with students was more intimate and connected than it was in a traditional classroom (*1*).

In Nanoscience for Teachers, our participants did adapt to the environment and used verbal immediacy behaviors and emoticons during online chats and forum posts. In general, the mood during the chat discussions was upbeat, as portrayed by positive comments and politeness gestures, such as by saying “Thank You ☺” when the guests answered teachers’ questions.

Coppola et al. also found that the managerial role requires a greater attention to detail and additional student monitoring (*1*). Faculty indicated they had to monitor student discourse and provide individualized feedback to students more often. Some found the level of monitoring “daunting” at times.

In our course, we did have to increase our student monitoring in a manner to make sure all teachers were engaged. The first author, as the main instructor of Nanoscience for Teachers, made sure to provide feedback and answer questions as soon as possible: within the same day they were posted. Whenever possible, graded work was returned to participants within the week after it was submitted. If a student did not login or complete assignments, the instructor sent them an email reminder and asked if there was anything preventing their participation that she could help alleviate. We found that it was important to provide feedback on assignments early and often, and to answer questions as soon as possible. The goal for giving prompt and immediate feedback was to ensure that participants felt as much of an immediate instructor presence as possible. Prompt instructor feedback is important in face-to-face classes, but we find is even more important for the online setting. Students can feel disconnected and as though they are not a part of a learning community if there is not enough interaction with the instructor in a distance learning course (*37*). Researchers have found a correlation between students’ perceived interactions with instructors and the average number of responses instructors made (*38*). Predictably, students feel they have more interaction with the instructor as the number of instructor responses to the student increases.

The instructor in the online setting also serves as an important model for course discourse. In the study of verbal immediacy behaviors in online courses by Rourke et al., the researchers compared the conference transcripts between two similar graduate-level online courses (*33*). They found that there was a greater “social presence” in the course in which the instructor was both an active participant in the discussion as well as a moderator. In the other course, the instructor served mainly as a passive moderator of the discussions (*33*). In our online course, as the instructors, we participated in the course in a variety of ways: making forum posts, responding to participant comments and questions, and interacting with the guest researchers in the weekly online chats. We were as much active participants in the course as we were leaders. In this way, we could

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help start the discussions and serve as models for the course communications. We found teachers were more engaged in the course communications after we began discussions and interacted with the participants. Picciano and coworkers found that instructor activity directly related to students' perceived learning (*39*). In their study, the instructor took on the role of "facilitator of learning." In their setting, the teacher was more of a guide while the students took an active role in the discussions. This role permitted the students to have a greater voice in the discussions and in their learning. Research indicated the students perceived high levels of learning using this approach. In our online course, we prompted the teachers for comments in the online forums and during the chat discussions, and then let the conversation flow naturally as others responded. In this way, our teachers had control over the direction of the discussion, so they could glean the information they desired from the experience.

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Interactivity with Peers

Much of the pedagogy behind learning in an online setting is based on constructivist learning theories, specifically social constructivism and social constructionism (*40–42*). These theories hold that the learning process occurs in a collaborative setting when the learner constructs something useful for others to experience. Essentially, learning is a social process involving the interaction among the learner, peers, and the instructor. So it follows that a successful online course should have ample opportunities for peer-to-peer interactions.

One important means of communication is the asynchronous discussion (forum posts and email, for example). As one would expect, the nature of online discussions can be different from face-to-face courses. It has been argued that online discussions can seem disjointed, less personal, and can more easily be misinterpreted compared to those in a face-to-face environment (See for example Sproull & Keisler (*43*)). In early studies of online chemistry courses, it was found that email as the only means for communication between students and the instructor is not a sufficient method for interacting (*44*, *45*). Students experiencing communication only via email felt less connected to their peers and had less sense of community (*46*).

Others counter that the online environment has potential for being "hyper-personal", or "richer." (*33*, *36*, *47*, *48*) Researchers studying the discussions in virtual classrooms find that often the online setting can provide students with more time to reflect on comments before typing a response (*49*, *50*). Also, participants create adaptations for conveying emotions typographically that can make up for the absence of physical cues (*51*). Students have reported experiencing more interaction with their peers when sharing in-depth online messages (*52*).

So there is potential for creating a rich and vibrant community in the computer mediated classroom. Though, as can be expected, this requires the buy-in of the participants. The amount of interactivity between peers depends on the frequency and the timeliness of the messages and responses posted in the online course (*53*). Jiang and coworkers found that the student perception of interactivity in an online setting was correlated with the average number of responses the students themselves made in the course discussions (*38*).

The perceived interactivity between peers is also influenced by the emphasis the instructor places on discussions (*29*, *38*, *54*, *55*). In the study by Hawisher and Pemberton, student comments were more connected and acknowledging of each other when the instructor required online discussions as a grade in the course (*55*). Grading of asynchronous discussions can take many forms; from the simple counting of the number of forum posts per student, to a detailed rubric that assesses the content, quality, and the nature of the student comment (*54*). In the study by Jiang et al., the authors found that students' perceived learning was positively correlated with the percentage of the final grade the discussions were worth (*38*).

In the first version of Nanoscience for Teachers, we did not place a great emphasis on the forum discussions. In the next version, we made posting in forums a larger part of the course grade, and we saw a large increase in the number of forum comments. In this version of the course, the teachers indicated the learning environment more closely matched their ideal preferences (*3*). Teachers also interacted with their peers through the final projects. The teachers uploaded their nanoscience teaching modules to the online course and then peer-reviewed them as part of the project grade. The final project is an example of social constructivist learning in action: the teachers shared something useful they created with others in the online community, and they benefitted from the project reviews of their peers.

In at least one recent study, however, grading group assignments did not make a significant difference to participation levels (*56*). Brindley and colleagues point out a variety of other factors that can lead to high levels of student-student interactions, specifically through group-work in online courses. They found that to ensure successful collaborative work, instructors should set clear expectations and instructions for participating, that assigned group tasks should be appropriate for a group and not better suited as an individual assignment, and that the timing of group assignments be such that students have gained a sense of the online community before forming a smaller work group. Bindley et al. also discuss the importance of learner autonomy, and ensuring that students have enough control over a task (assigning group roles, control over content and goal settings and group partners) so that their sense of responsibility and relevance of the task increases (*56*).

Others have discovered that too much forced interaction between students and peers may feel unnatural to participants (*57*). Biesenbach-Lucas reports that excessive forcing of discussion postings may stifle motivation to introduce new topics or alternative issues in online discussions. Students also indicated they would have preferred the instructor to post assignment prompts to stimulate the Web discussions, making them more structured and focused.

So far, much of the research discussed in this chapter concerns asynchronous, or "any time," discussions that occur over a longer period of time via forum posts or email. Synchronous, or "real-time," conversations have become more viable over the past decade with the advent of better Web technology and higher bandwidth capacity. One common tool for synchronous discussions is the online chat. Students and the instructor can discuss topics live in the chat, creating

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a greater sense of a community in the online course (*58*). In Nanoscience for Teachers, we held an online chat each week (see Table III). Chats were generally scheduled for later in the week (Thursday or Friday) in the early evening (4:00pm), when everyone could be online. For each chat, we invited a different guest nanoscience expert to discuss his or her research and answer any questions our teacher-participants had.

While live chats can be a positive part of an online course, if they are not organized they can seem frustrating and disjointed, often with fragmented comments and multiple conversations happening at once (*59*). In Nanoscience for Teachers, the first chat was a learning experience for participants (*3*). The instructor would begin the chats by introducing the guest researcher, and then ask if anyone had any questions. Often more than one person would jump in and type in multiple questions; the guest would take turns answering the questions, but it could be difficult to follow if there were interruptions by other participants. At subsequent chats, people learned to take turns and the conversation flowed more naturally and was easier to follow. For the second version of Nanoscience for Teachers, participants were asked to post their questions for the guest speaker in the online forums a day in advance of the chat. In this way, the speaker could prepare answers in advance and then at the chat, he or she could answer each question in order. If participants jumped in with any related questions everyone was on the same page.

Recently, a simple yet ingenious protocol for managing an online chat was published by Smith (*59*). His strategy was intended to "tame the chat beast" and make the synchronous discussions more natural and easier for participants to follow. He required students in his online graduate course to use special characters and symbols as conversation-change cues during the online chats. After the initial introduction by the instructor, if a participant had a comment or a question, they were to type "!" for a comment, or "?" for a question (similar to raising a hand in a face-to-face classroom). When a participant was typing, he or she should type in sentence fragments and hit 'enter' often, so others would read the idea as it unfolded, and not have to look at a blank window waiting for it all to be typed in at once. At the end of a participant's comment he or she should type three forward slash marks (///), letting everyone know the comment or question had concluded and giving someone else a chance for a turn. Smith also had clear rules for "chatiquette" (chat etiquette), that included no interrupting while another participant had the floor, taking turns for speaking, and no sidebar conversations (*59*). These rules are ideal for making the chat dialogue smoother and easier to follow, and do not require any expensive technology such as a microphone or headset.

Another means for synchronous communication in an online course is the Web conference, or "Webinar" or "Webcon." With current advances in technology, the Web conference has become a useful tool for online instructors. Some examples of commonly used Webinar software include Elluminate Live! (*60*), Adobe Connect (*61*), Ready Talk (*62*), and Wimba (*63*). Students have shown positive response to use of Web conferences in the online setting, and in some cases student performance can be improved compared to courses using asynchronous text-based lectures (*64*).

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Class size is also another aspect that influences peer (and instructor) interactivity in the online setting. Some have found that the optimal online class size is 15 – 20 students (*65*). In our online course, our largest class size in a semester to date has been 12 participants; this was a comfortable size, though we could probably expand to 20. If we had more than 20, we predict the design of the course would have to change. In a larger class size, the online chats might become more difficult to follow; not everyone would have a chance to ask the guest expert their question. In this case, we would probably move the discussions with the guest researcher to be completely asynchronous through the online forums, and occurring over the full week. This would allow more participants to interact with the guest, and the rest of the class could follow along with the discussion as it proceeds throughout the week. Grading would become more intensive; we might consider changing the nature of the online quizzes from essay-type questions to short answer questions that would be easier to grade for a larger class.

Interactivity with Content

Students in a computer mediated classroom will interact with the content as much as they interact with their peers and the instructor. There has been much research examining the many ways to ensure highly interactive course content. Janicki and Liegle reviewed a variety of instructional design studies and Web-based design research to create an inventory of ten important aspects for the effective design in an online course (*23*). Janicki and others have found that using a variety of presentation styles for course content and including multiple exercises and examples will allow the course to appeal to multiple learning styles (*23*, *66*).

Janicki and Liegle also cite research on the importance of letting students control their navigation through the course and their learning to a certain degree (*23*). In their online course model, students must read the learning objectives and key points for a topic initially, but then are free to decide the path for working through the key points. Through the hyperlinks in the course, the students can either view content with examples and exercises, or view only examples.

Some other important aspects pointed out by Janicki and Liegle include using a consistent layout and clear navigation throughout the course, providing help screens, and frequent testing. The latter can take the form of non-graded quizzes at the ends of tutorials or more formal graded quizzes and exams, utilizing a variety of testing formats (multiple choice, essay, short answer, matching). As discussed earlier, the course management system Moodle helped us organize our content into a meaningful layout, so that our teachers found it to be effective (*3*).

Conclusions

Just as in a traditional classroom, a successful online course is one that promotes high quality learning and provides an interactive environment in which participants are a part of a community that shares knowledge with each other. One of the first steps for designing the course is to choose content that is relevant

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for the participant. When choosing and uploading content, course developers should be sure to consider copyright protocols and follow the legal requirements for obtaining permission to use the material. The arrangement of content in the Web space is also important; the course should have a clear structure and straightforward layout so participants can easily navigate throughout the virtual classroom. A course management system, such as Moodle, is a helpful program for arranging and hosting the course online. Many of the features in a course management system help create an interactive environment for participants. In our course we used Moodle, which allowed for interactions with participants through the online chats, forums, and workshop activities.

According to constructivist learning theory, a crucial part of learning takes place when the learner constructs something useful for others to experience. Learning is a social activity, so it is imperative that the online course fosters high levels of interactivity among participants. The instructor plays important roles in the online setting, and some of these roles have shifted from those in a traditional face-to-face environment. Teachers in the virtual classroom must serve as models for course discourse, provide students with feedback earlier and more often, and increase their student monitoring to make sure participants are fully engaged. The actions teachers take impact student perceived learning in the online course; the more interactive the instructor is with the students, the more students perceive they learn.

In Nanoscience for Teachers, the first author, as the main instructor, made sure to provide students feedback and answer questions as early and frequently as possible. In this way, she created a presence in the online environment that the participants noticed and felt connected to, which helped the virtual classroom become a learning community.

Designing a course with high levels of interactivity among peers is also crucial. Increasing levels of peer interactivity can be challenging, and requires buy-in by all participants. Giving group assignments can also be effective, provided the assignment is appropriate for group work and students have some autonomy over the assignment and their learning. Studies show that using only email as means for course communications is inadequate. The instructor should encourage the use of forums within the course as well as email communications to direct asynchronous discussions. For real-time discussions, the instructor can use online chats or Webinars. Participants should follow guidelines for synchronous discussions and take turns asking questions and commenting so the conversation is organized and easier to follow.

There were many ways we ensured high levels of peer interactivity in Nanoscience for Teachers. One way was through our online chat discussions with guest nanoscience researchers. The online chat was a way to allow instant communication, which increased the sense of a classroom community. We found that after an initial period of getting familiar with the chat process, participants took turns asking questions of the guest researchers and exhibited appreciation for speaking with the guests during the chat dialogs. Peer-reviews can be another way to have participants interact and provide crucial feedback to one another. As a final project in our course the teachers created nanoscience teaching modules to take back to their own classrooms. In this way, they were creating something

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useful for their profession from the experience. This made the content more relevant and meaningful for their lives. The teachers shared their modules with each other and provided peer feedback as part of the final project grade.

Our research has shown that Nanoscience for Teachers has been very effective for creating an online learning community, for conveying content, and for enabling teachers to apply what they have learned in their own classrooms (*3*, *7*). We continue to make updates, and next we will replace the online chats with Webinars, to allow our participants to share PowerPoint presentations and to transmit audio over the Web. The course will next be offered through Central Michigan University, where the first author now works. Creating a successful online course is not an easy task, but when the developer is aware of each of the aspects discussed in this chapter, the course will begin to take shape. Similar to architecture, if a course developer builds a strong foundation, the online course is more likely to become a pillar for educational success.

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Chapter 13

Instruction Online: Core Components for Re-Use

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This chapter reflects on our development of technology for chemical education over the past one and a half decades. We begin by identifying those features of educational components that hold the greatest promise for education. Although there are many advantages to be gained by moving existing instructional approaches online, via online lectures and practice problems, the greatest potential likely lies in using technology to fundamentally change the nature of the explanations and practice. Digital libraries have the potential to enable such fundamental change by engaging a large community of educators in the creation and refinement of educational components. From a technical perspective, this requires the use of technologies that allow instructors to easily create and modify interactive content. From a broader perspective, this requires using the experience gained from classroom use of the components to iteratively improve the content. We close this chapter with four design principles that have emerged from our past work, which we illustrate by showing how these principles have influenced our most recent curriculum development efforts.

Introduction

The use of technology in education has the rich potential of encouraging the community of educators and professionals to re-think the fundamentals of instruction. When textbooks were the primary vehicle for collecting and disseminating information, the cost and time involved in re-structuring the content and instruction was so high as to drastically limit the number of design participants and the number of revisions. But with current online technology, the potential for many scholars in chemistry to contribute new vital information has blossomed. By providing a community space for authoring and distribution of smaller pieces of instruction (components and modules), digital libraries can encourage larger participation. The technology itself can, however, act as a limiter of such participation, both because of the time required to acquire the expertise and, for many current technologies, the large time investment required to develop interactive materials. This paper is a reflection on our development efforts over the past decade and a half, with the goal of identifying critical features of educational components and design principles for developing new components.

The materials we have developed include virtual labs, scenario based learning activities and tutorials on challenging aspects of chemistry. These are housed in the ChemCollective digital library and are made freely available for noncommercial use. Our discussion considers only technologies for learning and instruction, as opposed to assessment. While detailed definitions of instructional parts need to be developed and agreed upon, we will focus on two elements: the component and the module. In broad terms, a component is the smallest piece of instruction that it would make sense to store as an individual item in a digital library. Module refers to a systematic collection of components designed to meet a specified learning goal. Student interaction in a module consists of a sequencing of components.

Some of the strongest benefits of a digital library result from *repurposing* and *iterative improvement* of components. *Repurposing* is use of a component in a context other than its initial target, for instance, through re-sequencing of components to get different instructional paths or by developing a different cover story. One of our design strategies, aimed at ensuring repurposeable components, is to target multiple contexts in the initial design of the components. *Iterative improvement* of components is the ability for the community to discuss, assess, modify and improve a component such that, over time, it can best meet the needs of the target audiences. A design strategy for supporting such iterative improvement is to provide instructors with a means to author or edit interactive components in a way that does not require programming expertise.

There are two dimensions along which to consider the instructional components in a digital library (Table 1). The first dimension is explanation

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versus practice. At one extreme of this dimension lies instructional explanations (*1*), which provide a means for students to acquire knowledge. At the other end of this dimensions lies practice, which provides a means for students to deepen and refine their knowledge. These dimensions are not meant to be categorical, but rather form a continuum. Modules will necessarily go back and forth between explanation and practice. Components may also lie between the two extremes. For instance, consider a component that poses a question to a student and then gives feedback that may include an explanation of a concept as part of reinforcing or correcting the student response. Such a component blends practice with instruction and so can be viewed as lying intermediate along the instruction-practice dimension.

The other dimension is the degree to which the instructional component fundamentally changes the nature of the explanation or practice. At one extreme of this dimension are approaches that change only the modality of the delivery or interaction. Examples include online videos of classroom lectures, or online question banks constructed from a textbook's end-of-chapter exercises. Such changes in modality can have significant impacts on instruction, for instance by allowing 24 hour/7 day access to lectures, by promoting more regular and better spaced practice, and by providing instant feedback on student responses. In each of these cases, the fundamental nature of the instruction remains that which traditionally occurred in the classroom or during paper-and-pencil practice. As one moves along this dimension, the component fundamentally alters the nature of the explanations or practice. Perhaps the greatest potential of technology for education is that it encourages the community to step back and re-examine the instruction process from the ground up. Such efforts may lead to explanations that follow an entirely new learning trajectory, or practice in which students engage with chemical concepts in an entirely new way. For instance, our virtual lab uses technology to provide new modes of practice with chemical concepts. Motion along this dimension does not necessarily involve the use of technology in the components themselves. For instance, we have developed new explanations for chemical equilibrium that do not rely on a technical mode of delivery. But by aiding dissemination and iterative improvement of such content, digital library technology is nevertheless an important enabler for such developments.

Our discussion is based primarily on the following curriculum development projects.

Virtual Lab Collection A collection of activities for our virtual lab (see *Virtual laboratory*), browsable by course topic and labeled according to activity type and our estimate of the difficulty level of the assignment. These are among the most popular items in the ChemCollective digital library. Since the software is freely distributed, usage is not fully monitored, but the virtual lab was run over 200,000 times from our Web site last year and downloaded over 40,000 times.

Table 1. Categorization of our instructional components along two dimensions. Horizontal: The degree to which the component provides instructional explanations versus supporting student practice with concepts. Vertical: The degree to which the component is a modality change on traditional instruction or practice, as compared to a fundamental change in the nature of the instruction or practice

	Explanation	*Practice*
Modality change	Videos of instructional explanations	Online practice questions
Fundamental change	Molecular-level visualization Interdisciplinary approaches	Virtual laboratory Molecular-level simulation

Stoichiometry Course An online review course in stoichiometry aimed at students who are about to enter college chemistry and need a review of this important foundation material. The course is set in the context of arsenic contamination in the groundwater of Bangladesh and contains 15 modules ranging from the mole and molecular weight up through reaction stoichiometry, empirical formula and limiting reagents. Modules typically start with an instructional explanation covering the relevant concepts, followed by practice questions, and then either a virtual lab or more extensive problem solving tutor. It is available as both a full online course [https://oli.web.cmu.edu] or a collection of tutorials [http://www.chemcollective.org/tutorials.php].

Equilibrium Course An online course that implements a new instructional approach to equilibrium. By analyzing current instructional approaches and conducting student interviews, we identified key concepts and problem-solving strategies that were left implicit in traditional instruction. We then designed instruction that made these concepts and strategies explicit. A live classroom implementation of this instructional approach more than doubled student performance on difficult problem types (*2*). Our equilibrium module implements this new instructional approach, either as an online course [https://oli.web.cmu.edu] or a collection of tutorials [http://www.chemcollective.org/tutorials.php].

Core Ideas in Molecular Science (CIMS) A collection of interdisciplinary instructional modules that are appropriate for use in discipline-specific courses, yet designed to help students draw connections across multiple disciplines. We close this chapter by using our approach to this most recent development effort to illustrate the design principles we have developed in the process of our decade and a half of work in this area.

We have conducted a variety of research studies on most of these efforts (*2–8*). These studies range from classical randomized experiments, to quasi experiment, to observations of student problem solving and examination of novice-expert contrasts. For example, in one study of the stoichiometry course we compared the online course to a parallel paper-and-pencil version. The paper-and-pencil version did not contain the scenario or the virtual labs. The problem solving

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practice was carefully constructed to be as parallel as possible to the online course, using the same problems but without the hints and feedback made possible by the technology. Instead, for each topic, students were given (i) a worked example that showed the problem solving actions side-by-side with the rationale for and justification of these actions, (ii) a worked example that included only the actions, with a prompt asking students to fill in the justifications and (iii) a set of practice problems with only a numerical answer provided for students to check their work. This paper-and-pencil version competed well with the online version, suggesting that well constructed non-technical implementations can still be quite powerful for learning. However, in the online version increases in activity with the virtual lab led to corresponding increases in student performance. We also note that the learning assessment in this controlled study focused on traditional problem solving, with some conceptual questions on stoichiometry. Additional features that were covered only in the online course, such as the application of stoichiometry to real world situations, or the design and implementation of experiments that use stoichiometry, were not assessed (*5*).

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Components

Online Instructional Explanations

An instructional sequence typically requires components that explain the concepts in an expository manner. Before the advent of interactive digital technology, such expositions were done either through text and static images, as in textbooks, or through live lectures and physical demonstrations. Although current technology is quite far from providing the rich experience and learning benefits of human discussion, online content may be competitive with lectures and even lectures that provide motivating live demonstrations. Given the potential for the community as a whole to iteratively improve online content, online explanations have the potential to surpass live performances. In this section, we first discuss various common means to move text and lectures online. We then discuss our past workflows for creation of online explanations, and how experience with these workflows informed the design of our EX_2 system for creation and delivery of explanations.

Moving Text Online

Moving text and static images online has a number of advantages, connected to the ease with which the content can be created and modified. The dramatic success of Wikipedia illustrates the ease with which a community can create and iteratively improve such content. The ChemEd DL's online textbook (*9*) has the potential to bring this iterative improvement to explanations in chemistry. Such content is also easily repurposed. In addition to simply cutting and pasting the content in different organizations, hyperlinks allow the text to be organized in multiple ways. For instance, the WikiHyperglossary (*10*) allows glossary definitions and other content to be linked automatically to words on a page, via links generated and automatically maintained by the system. Our equilibrium course uses hyperlinking to support two organizations of the components: a recommended first pathway through the material for initial exposure to the concepts, and a conceptual organization for studying and review of the material.

A potential disadvantage of moving text online is that it may make the material more difficult to read for long periods of time, to add annotations and notes, and to browse through quickly (as compared to flipping pages of a textbook).

Moving Classroom Lectures Online

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Moving classroom lectures online is a challenge that has been the target of a number of evolving technologies. These typically function as online videos, in that they present images and audio in a time sequence. Advantages to the student include instant access at any time, and the ability to self-pace the lecture through pausing or replay. A potential disadvantage, relative to live lecture, is the inability to interact with the lecturer and ask questions.

We have used a number of approaches for creating and delivering content that essentially function as an online video. For our stoichiometry course, we used Adobe Flash and Apple FinalCut Pro to create multimedia presentations that combine text, images and some animations with spoken audio. Our current view is that any benefits resulting from this approach (a clean professional look, highly legible contents, etc) are offset by the time and effort involved in authoring. Even more problematic is that the time and difficulty associated with modifying such contents limits their iterative improvement, both by the original authors and by the larger community.

Filming a live lecture is the easiest way to create online lecture content. For instance, we created an online course by combining videos of live classroom lectures with other components (written lecture notes, worked examples, practice questions and assessments) [http://oli.web.cmu.edu/jcourse/webui/guest/look.do?section=chemvid]. The ease of production is relatively high, but the quality of the outcome suffers from the videos not being iteratively improvable, even by the initial creator.

The Explanations with Examples (EX_2) System

Given the large proportion of our development time that we spend developing online explanations, we are attempting to develop improved authoring approaches through a set of tools we are calling EX_2 for “explanations with examples”. EX_2 is based on an analysis of our previous workflows, and a working hypothesis for the benefits of video over text (or static) explanations.

One of our earliest work flows was that used to create the multimedia presentations for our online stoichiometry course. We began with a film of an explanation being delivered at a blackboard. From this we created a written script that, once vetted by all project participants, was read aloud to form an audio track. Multimedia authoring tools were then used to assemble graphics on top of this audio track, which in most cases reflected what appeared on the blackboard during the initial filming. Although this leads to a product that looks quite professional, this approach has some serious disadvantages. One of the more problematic issues is the difficulty of carrying out a complex explanation on the limited screen real estate of a non-scrolling stage. (A similar problem can arise in attempting to put a complex explanation into PowerPoint slides.) The lectures also followed a linear timeline and were not customizable. But perhaps the most limiting aspect of this mode of creation is the large amount of effort and time required to create or edit the final product. (Initial creation time was about 10 hours per video, with each video being 5 to 10 minutes long.)

That experience led us to develop more efficient workflows, such as creating a screen capture of writing on a tablet computer while simultaneously recording audio through a microphone, using CamtasiaStudio [http://www.camtasia.com]. Such an approach worked well for quickly creating rough drafts, however it was difficult to speak and write fluidly and to avoid errors in a long, screen-capture session. More polished results are obtained by first writing out all items that are to appear on the screen, and then cutting and pasting these into the screen capture region while speaking. To obtain even higher quality, we first type out a script, record this as an audio track, and then play back and capture this audio while cutting and pasting objects into the screen capture window. This is considerably faster than the full flash production mode, taking about 2 to 3 times as long as it would take to prepare and deliver an in-person lecture. Nevertheless, it restrains us to a linear video mode, produces content that is difficult to edit (even a simple change requires recapturing a large portion of the video), and delivery can require considerable bandwidth. Nevertheless, we have found this technique to be the most convenient means to author usable explanations and worked examples with existing tools. We have used this approach to create tens of such videos that complement our classroom teaching by providing students with videos that cover particularly difficult concepts.

In addition to analysis of the above workflows, our EX2 system is based on a working hypothesis of the benefits of a live explanation (be it video or non-interactive classroom lecture) over text. Our hypothesis is that the benefits result from combining a permanent record of key features of the explanation (the items written on the blackboard, or that appear on the computer screen) with transient information (the spoken words of the lecturer, or the audio track of a video). The transient information is needed to understand the rationale for the item written on the blackboard, but once that item is understood, the highly summarized version that remains on the blackboard is sufficient for recall. For complex explanations, this separation of a permanent trace from transient information makes it possible to see the forest for the trees.

From an authoring perspective, the goal of the EX2 system is to support construction of explanations through a process that closely resembles the familiar mode of a blackboard lecture. Items that would usually be written on the blackboard are created with a tablet computer, or other graphical tool, and deposited onto the permanent visual stage. Supporting material that would usually be spoken in the lecture is then attached to these items as audio. (Optionally, a text version of the audio track can be provided, to serve as subtitles for users

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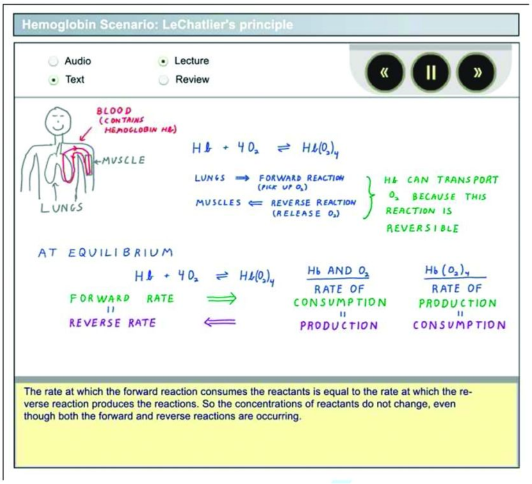
where audio is not convenient or possible.) The creation of the graphical objects and the recording of the audio track are done separately, since it is difficult to simultaneously write neatly and speak clearly without making mistakes.

The outcome of the authoring process is a sequence of graphical objects, with associated audio or text annotations, that constitute a single flow through the explanation. The sequence is specified in an XML file that contains pointers to the graphics that appear on the permanent stage and the associated audio or text. The ease with which the author, or any community member, can modify and iteratively improve the content approaches that of an HTML page. The EX_2 viewer, discussed below, positions things on the screen dynamically based on the XML file, and so objects can easily be modified, inserted into, or deleted from, the flow of the explanation without the need to modify any other portions of the content. The visual stage is a single scrollable window, eliminating the need to break the explanation onto individual computer-screen sized pages.

The student views the resulting content through the EX_2Viewer, which has both play and review modes (see Figure 1). In play mode, the student views the materials in progression, with optional replay and branching. In review mode, all items are visible on a scrollable stage, and clicking on any item brings up the associated transient information, either as audio or text. Review mode therefore behaves as though the student walked into class at the end of the lecture and could instantly call up what was said about any written item. These modes are provided to support students as they initially learn the material, and later as they review it while engaging in practice problems or studying for an exam. The EX_2 system was used to create the explanations for our equilibrium module.


Hemoglobin Scenario: LeChatlier's principle
○ Audio
● Text
● Lecture
○ Review
«
II
»
BLOOD (CONTAINS HEMOGLOBIN Hb)
MUSCLE
LUNGS
Hb + 4O2 ⇌ Hb(O2)4
LUNGS ⟹ FORWARD REACTION (PICK UP O2)
MUSCLES ⟸ REVERSE REACTION (RELEASE O2)
Hb CAN TRANSPORT O2 BECAUSE THIS REACTION IS REVERSIBLE
AT EQUILIBRIUM
Hb + 4O2 ⇌ Hb(O2)4
FORWARD RATE = REVERSE RATE
Hb AND O2: RATE OF CONSUMPTION = PRODUCTION
Hb(O2)4: RATE OF PRODUCTION = CONSUMPTION

The rate at which the forward reaction consumes the reactants is equal to the rate at which the reverse reaction produces the reactions. So the concentrations of reactants do not change, even though both the forward and reverse reactions are occurring.

Figure 1. The EX_2 Viewer

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Research on worked examples suggests that effort invested in creation of such content can lead to substantial learning gains. Well designed worked examples, while not interactive, have been shown to yield learning results that rival those of interactive tutors requiring considerably more development effort (*11–15*). Students who learn best from worked examples are those that engage in a set of attentional behaviors that have been labeled “self explanation” (*14*, *16*, *17*). We plan to add features to the EX2 viewer that may promote close attention to the details of the example. In particular, we would like to add prompts with standardized labels such as: *strategy* for how a step is advancing us along the problem solving strategy, *validity* for why this step is allowed under the constraints of the domain, and *alternatives* for steps that would also be valid at this point in the problem solving. These are likely the types of questions learners would ask themselves while engaging deeply with a worked example, and so such prompts may help students learn better from worked examples. There is also evidence that reflection on the meaning of the practice leads to both greater retention of content and better forward learning (*18*), and prompts for this manner of reflection may also be inserted. More generally, a flexible authoring and delivery tool such as EX2 would enable the community to start from an initial attempt at an instructional explanation and iteratively improve it by, for instance, altering the explanation, presenting a range of examples, adding alternative problem solving pathways, and inserting prompts that promote various styles of reflection.

Online Practice Questions

Online practice questions are the current most common way to provide students with practice online. This is not surprising, given that in traditional instruction, the end-of-the-chapter questions and problem solving activities are the primary mode of practice. The advantages to moving such questions online include: requiring students to stay on track with the course by having regularly scheduled graded homework, providing feedback to students based on their responses, and providing more practice opportunities via parameterized question types. In addition, feedback to instructors, in the form of student performance on various questions, may allow instructors to better tailor their instruction to student needs. In most cases, the questions are similar to those of textbooks, and so such online homework systems correspond strictly to changes in modality. Indeed, WebAssign allows instructors to assign online homework that contains questions taken directly from their course’s assigned textbook [http://www.webassign.com]. It is a given that distributed practice is far more effective than massed practice and online environments can help press students to engage in this type of practice; however the issues of practice are more complex than just when it is done.

In creating online materials, we have found it useful to consider two general categories of practice questions. One category is questions that serve as initial practice with the concepts. These are study aids that should provide high levels of scaffolding and feedback. The second category is questions intended as summative assessment of student knowledge. By assigning a portion of the course grade based on such summative assessments, we can encourage students to study in preparation for the assessment. Our analysis of a semester-long introductory college course indicated that such preparation is an important learning opportunity in courses (*3*), and as we move part of our instruction online, we have retained summative exams as a way to promote such study behavior.

Authoring Systems for Practice Questions

It is useful to consider the range of functionalities provided by various approaches to creation and delivery of practice questions. These span a broad range, from systems that support a few well specified question types, up through flexible cognitive tutors that compare student actions to a computer model of problem solving in order to provide highly-contextualized hints and feedback.

One category of question authoring systems are those that support standard question types, such as those in the IMS QTI specification (*19*). Such question types include, for instance, multiple-choice questions with feedback attached to each of the responses and questions that accept a numerical response within some specified range. Such well specified question types make it easier to: create user friendly authoring tools; support question management systems that, for instance, create randomized student assignments by pulling questions from a question bank; and allow transfer of questions between different course management systems such as Blackboard, WebCT and Moodle. We have found these styles of questions to be useful for summative assessments, but have found them less useful for providing practice.

More flexibility can be obtained by systems that allow free-form placement of user-interface (UI) components such as drop-down lists, radio buttons, and text boxes for entry of numeric answers. For instance, the Open Learning Initiative at CMU has developed a collection of Flash based tools [http://www.cmu.edu/oli] that allow UI components to be mixed with text and images on a multimedia panel (see Figures 2 and 3). This provides considerable flexibility to the author. The author can break a computation into multiple steps, or combine UI components to allow more free-form input. Feedback is provided through a sequence of hints attached to each UI component. When a user clicks the hint button in the upper right corner, the first hint associated with the current UI component is shown, along with a button that allows them to view the “next hint”. In most cases, we provide hints that walk the student through the task associated with that particular UI component. The first hint is a restatement of the goal of this stage of the problem solving, intermediate hints give partial information that guides students towards the correct response, and the last hint is a “bottom out” hint that provides the answer. Reading through all of the hints thereby provides a fully worked example. Feedback on student responses can also be attached to each UI component. Our feedback on correct responses typically includes text that reinforces the key concepts, while feedback on incorrect responses provides details regarding the student error.

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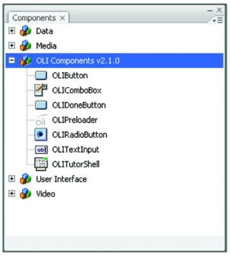
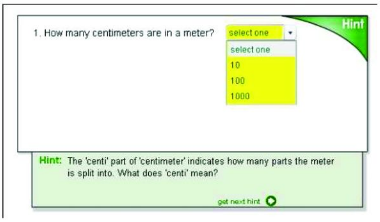


Figure 2. OLI Flash Based Components shown as they would be selected and dragged onto a user-interface panel.



1. How many centimeters are in a meter?

Hint: The 'centi' part of 'centimeter' indicates how many parts the meter is split into. What does 'centi' mean?

Figure 3. An example tutor created with the OLI Flash Based Components of Figure 2.

A primary limit on this technology relates to sequencing. The author assigns a sequence to the UI components, which determines the focus behavior of the UI components. (Here, focus is used in the computer interface sense that any key strokes are sent to the UI component that currently has focus.) As the user completes the task associated each UI component, the focus shifts to the next component in the author-specified sequence. The user can also click on any UI component at any time, and see the hints and feedback associated with that component. The hints and feedback depend on the current UI component, but do not consider the pathway the student followed to get to that component.

The Cognitive Tutoring Authoring Tools (CTAT) allows hints and feedback to be customized for various pathways through a problem solving activity [http://ctat.pact.cs.cmu.edu] (*20*). CTAT uses a behavior recorder to monitor interactions of the user with the user interface. The behavior recorder generates a graph, in which nodes correspond to a different state of the user interface, and edges correspond to actions that transition the user interface from one state (or node) to another state (or node) (See Figure 4). Hints and feedback can be attached to any edge of the behavior graph. In the authoring process, the author demonstrates various anticipated pathways through the problem, including both correct and incorrect pathways, and attaches hints and feedback to the resulting graph. The resulting tutors have been named pseudo-tutors since the user experience is similar to that of a full cognitive tutor (*21*). The distinction is that full cognitive tutors have an underlying cognitive model of student problem solving that makes it much easier to generate alternative forms of the problem and to make additional tutors. The distinction between pseudo and cognitive

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tutors is therefore primarily on the authoring side, and CTAT provides tools that aid development of a cognitive model from a set of pseudo tutors, providing a potentially efficient means to creation of full cognitive tutors.

We have developed a set of pseudotutors for stoichiometry that cover dimensional analysis, moles, and molarity. [http://ctat.pact.cs.cmu.edu/inc/stoichiometry-tutor.php] Overall, however, we have found few cases where the sequence-specific scaffolding enabled by a behavior graph is necessary and so the bulk of our practice questions use the much simpler approach of providing feedback based only on the component that has the current focus.

As one moves from questions that have a standard format, such as the IMS QT specification, up towards pseudo-tutors, one achieves flexibility at the expense of generating materials that may be more difficult to repurpose and iteratively improve. Open source, stable, authoring tools for the more advanced question types discussed above may, however, make it possible to utilize such question types without hindering reuse.

In some cases, we have however found it useful to simply hard code the functionality into JavaScript, since this allows more flexibility with regards to user-interface construction. In particular, we have found JavaScript to be convenient for creating fall-back tutors, in which students are first given a question regarding a multi-step computation such as that involved in limiting reagent or empirical formula problems. If the student needs a high level of support, the interface changes dynamically into one that provides step-by-step guidance (Figure (*5*)).For such tutors, JavaScript has the advantage of easily allowing the region of the screen on which the tutor resides to change dynamically. The added flexibility comes at a cost to reuse, since modifications require direct editing of the JavaScript code and so requires programming expertise.

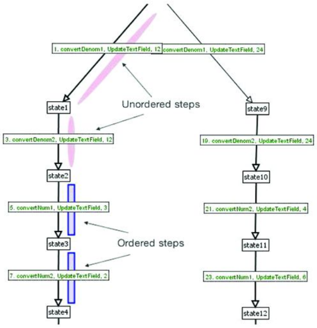
1. convertDenom1, UpdateTextField, 12
convertDenom1, UpdateTextField, 24
Unordered steps
state1
state9
3. convertDenom2, UpdateTextField, 12
19. convertDenom2, UpdateTextField, 24
state2
state10
5. convertNum1, UpdateTextField, 3
21. convertNum2, UpdateTextField, 4
Ordered steps
state3
state11
7. convertNum2, UpdateTextField, 2
23. convertNum1, UpdateTextField, 6
state4
state12

Figure 4. An example behavior graph generated from the CTAT system

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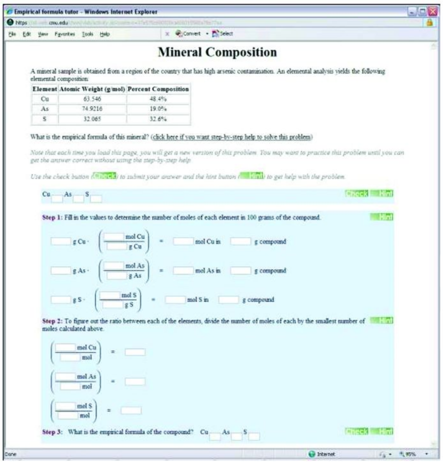
Empirical formula tutor - Windows Internet Explorer
https cmu.edu
File Edit View Favorites Tools Help
Convert Select
Check
Hint
Done
Internet
95%

Mineral Composition

A mineral sample is obtained from a region of the country that has high arsenic contamination. An elemental analysis yields the following elemental composition:

Element	Atomic Weight (g/mol)	Percent Composition
Cu	63.546	48.4%
As	74.9216	19.0%
S	32.065	32.6%

What is the empirical formula of this mineral? (click here if you want step-by-step help to solve this problem)

Note that each time you load this page, you will get a new version of this problem. You may want to practice this problem until you can get the answer correct without using the step-by-step help

Use the check button (Check) to submit your answer and the hint button (Hint) to get help with the problem.

Cu ☐ As ☐ S ☐

Step 1: Fill in the values to determine the number of moles of each element in 100 grams of the compound.

☐ g Cu · (☐ mol Cu / ☐ g Cu) = ☐ mol Cu in ☐ g compound

☐ g As · (☐ mol As / ☐ g As) = ☐ mol As in ☐ g compound

☐ g S · (☐ mol S / ☐ g S) = ☐ mol S in ☐ g compound

Step 2: To figure out the ratio between each of the elements, divide the number of moles of each by the smallest number of moles calculated above.

(☐ mol Cu / ☐ mol) = ☐

(☐ mol As / ☐ mol) = ☐

(☐ mol S / ☐ mol) = ☐

Step 3: What is the empirical formula of the compound? Cu ☐ As ☐ S ☐

Figure 5. The Empirical Formula Tutor showing the initial entry form for the student response (upper shaded box) and the fall-back scaffolding (lower shaded box) provided when the student needs additional help.

Virtual Laboratory

The practice questions we described use technology to provide scaffolding that is responsive to the student’s current knowledge and that fades as the student becomes more familiar with the material. However, this is primarily a modality change since the nature of the practice is similar to that of traditional textbook problem solving. Our virtual lab provides a more fundamental change to the nature of the practice, by allowing students to apply their formal knowledge to the design and implementation of chemical experiments (Figure 6). Students are given tasks that require them to design procedures and collect and analyze data. The affordances of this simulated environment are carefully designed to allow students in an introductory course to engage in this type of authentic activity. Experiments can be done much more quickly than in a physical laboratory, students can immediately see the contents of any solution (chemical species and their amounts), and in some cases fictitious chemicals are used to make the simulation easier to understand than an actual chemical system. However, we want to emphasize that the contrast of interest here is between end of chapter exercises and online practice activities, not between wet lab experiences and online ones.

Practice in the virtual lab is intended to be more authentic than that provided by traditional paper-and-pencil problem solving. Here, authentic means closer to the activities of practicing chemists. Our analysis of the domain of chemistry found that the primary activities in which chemists engage can be divided into three top-level categories: *explain, analyze* and *synthesize* (*22*). The virtual lab allows students to *explain* what is happening in a chemical system (e.g. determine what chemical reaction is taking place and why), *analyze* samples (e.g. determine the amount of arsenic in a sample of drinking water) and *synthesize* solutions with

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desired properties (e.g. create two solutions that when mixed together will lead to a target increase in temperature). Our virtual lab activities are meant to be authentic in the sense of reflecting the activities of practicing chemists. However, they are not necessarily intended to be authentic in the sense of being a replica of the real world.

The original motivation for the virtual lab was to embed the procedural knowledge of the course in a context that highlights its utility, such that students learn not only how to do a procedure, but also when to do it. This approach is supported by both Anderson's "Adaptive Control of Thought−Rational" (ACT-R) theory (*23*), which models learning as a series of production rules (e.g., if X, then do Y), with the X or condition component being just as important as the Y, and by the work of Lehrer and Schauble (*24*), which emphasizes the deep connections between developed procedures and core authentic questions within a domain. Observations of student problem solving showed another benefit of these problem types: that of helping students move beyond shallow problem-solving strategies (*25*). In particular, a useful but potentially superficial strategy for word problems is to categorize the given and requested information and then find equations that relate the information. For instance, a calorimetry text problem may give a measured change in temperature (ΔT given) and ask for the heat of the reaction (q requested), for which a student may identify $q = m\ C_p\ \Delta T$ as an appropriate equation. This strategy will not work on an activity that requires design of an experiment to measure the heat of a process. Experimental design requires deeper reflection, since the student must realize that this equation represents an experiment in which a temperature change is used to measure heat. Our observations show that students find the experimental design problem considerably more difficult than the text problem, suggesting that this connection between equation and physical process does involve additional learning.

As an example of the new forms of practice enabled by the virtual lab, consider one of our virtual lab activities that deals with the concept of limiting reagents. A student's practice with this concept typically centers around learning a standard computational procedure. Our "unknown reaction" virtual lab activity provides a different mode of practice. Students are given four unknown chemicals (A, B, C, and D) and are asked to design and perform experiments to determine the reaction between them (i.e. $A + 2C \rightarrow 3B + D$). We found that roughly 50% of students in our course misinterpreted the results of their experiments in a way that revealed fundamental conceptual misunderstandings (*8*) . When these students mixed A with C and found that A remained in the solution, they concluded that A must be a product of the reaction, as opposed to left over reactant, and wrote an equation such as $A + C \rightarrow B + D + A$, in which A is both a reactant and product of the reaction. Since this group of students has high proficiency in limiting reagent calculations, this result indicates that it is possible to be proficient in the algebraic procedure while still missing core aspects of the underlying concept. (The system provided immediate feedback that pointed out the conceptual nature of this error.)

The virtual lab was designed as a tool that instructors and curriculum developers could use to develop a broad range of activities. This is done by allowing the simulation to be configured via an XML file. The underlying simulation assumes all reactions go immediately to equilibrium, but is otherwise quite general. Thermochemistry is simulated in a general manner, such that reactions give off and absorb heat appropriately, and shift in response to temperature changes. Color of solutions is also handled through a fairly general scheme that can handle mixtures in a reasonably accurate manner.

The XML configuration file specifies:

- **Chemical species and reactions.** This allows authors to add new chemicals to the lab by specifying their thermodynamic properties (heats of formation and standard entropies) and the chemical reactions in which these species participate. These can include fictional materials, such as acids with randomly generated dissociation constants (for unknown identification activities) or idealized biological molecules such as proteins and drugs (for use in activities that are set in biological contexts).
- **Solutions.** The virtual lab stockroom can be configured to contain any desired solutions. This process is similar to setting out starting materials for a physical lab.
- **Viewers and instruments.** This allows the author to control access to instruments, such as the pH meter and thermometer, and viewers, such as the list of all chemical species in a solution and their concentrations. For instance, an unknown-acid activity would necessarily need to turn off the chemical species viewer. Access to the pH meter could be provided, or withheld if the author wants students to use a pH indicator such as phenolphthalein.
- **Transfer bar.** The virtual lab provides three means by which students can transfer chemical solutions between containers. The first is "precise transfer" in which students type in a specific volume. This is useful if the goal is to focus student attention on the chemistry without paying attention to experimental technique. The second is "realistic transfer" in which the volume transferred depends on how long an onscreen button is depressed. This is calibrated such that the attainable accuracy reflects that possible in a real lab. This requires students to use reasonable glassware, such as a buret for a titration. The third is "significant figures transfer", which is similar to precise transfer except that students must enter the desired volume using the number of significant figures possible with the given glassware. This mode of transfer was suggested by a community member and assessment by that community member indicated that this mode was more substantially effective in teaching the concept of significant figures than any of their extensive previous attempts (*26*).
- **Activity Description.** An HTML description of the activity can be included, which the student can view from directly inside the virtual lab.

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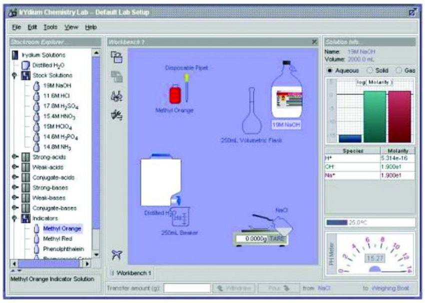
IrYdium Chemistry Lab – Default Lab Setup
File
Edit
Tools
View
Help
Stockroom Explorer...
Irydium Solutions
Distilled H_2O
Stock Solutions
19M NaOH
11.6M HCl
17.8M H_2SO_4
15.4M HNO_3
15M $HClO_4$
14.6M H_3PO_4
14.8M NH_3
Strong-acids
Weak-acids
Conjugate-acids
Strong-bases
Weak-bases
Conjugate-bases
Indicators
Methyl Orange
Methyl Red
Phenolphthalein
Methyl Orange Indicator Solution
Workbench 1
Disposable Pipet
Methyl Orange
19M NaOH
250mL Volumetric Flask
Distilled H_2O
250mL Beaker
NaCl
0.0000g
TARE
Workbench 1
Transfer amount (g):
Withdraw
Pour
from NaCl
to Weighing Boat
Solution Info...
Aqueous
Solid
Gas
log(Molarity)
0
-5
-10
-15
25.0°C
PH Meter
0
2
4
6
8
10
12
14
15.27

Name: 19M NaOH
Volume: 2000.0 mL

Species	Molarity
H^+	5.314e-16
OH^-	1.900e1
Na^+	1.900e1

Figure 6. Screenshot of the virtual lab

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This functionality provides authors with considerable flexibility in the design of virtual lab activities. The configuration is specified in an XML file. The XML file can be altered with any text editor; however, one must adhere to a fairly rigid set of formatting rules. To make it easier to configure the lab, we also created a virtual lab authoring tool that provides a graphical tool for configuring the virtual lab. This authoring tool saves the configuration to the required XML format. We have found, however, that the XML file is sufficiently easy to edit directly that most users either opt to do so, or simply send us all the required information and we create the configuration file.

Feedback on virtual lab problems is provided by the JavaScript question system discussed above (see *Authoring systems for practice questions*). A single Web page contains both the virtual lab java applet, and a JavaScript question form that provides hints and feedback. Randomized parameters, such as the identity and concentration of an acid for an unknown acid activity, are passed to both the virtual lab (through the XML configuration file) and the JavaScript question form. Students are typically given 3 attempts at entering their answer, after which they must reload the Web page and so are assigned a new randomly generated sample. The hints do not currently consider the actions the student has taken in the lab, and feedback to student responses is based only on the response itself. We are currently working on ways to provide feedback that is based on actions carried out in the lab (*6*).

Our use of a flexible, highly configurable, simulation to promote reuse has been quite successful. Of the 117 virtual labs in the current collection, 56 were contributed by 11 different user groups. A broad author base helps ensure that the activities can meet the needs of a diverse range of classrooms, including laboratory courses where virtual activities have been used as pre-lab assignments and to teach significant figures (*26*). Other projects that use configurable simulations to promote reuse include the physlets project [http://webphysics.davidson.edu/applets/applets.html], Interactive Physics 2000 [http://www.design-simulation.com/IP/] and the AgentSheets tool [http://www.agentsheets.com/]. Sharing of Mathematica and Maple worksheets may be taken as a very advanced example, in which the software tool is very highly configurable.

Molecular Level Visualization and Simulations

Another potentially powerful technology for both online explanations and practice is molecular level visualization. Such visualization is a major theme of chemical education. Here, we briefly describe what we learned from using molecular diagrams in our online equilibrium course. In the following section, we discuss how this has informed our design of a tool aimed at providing a general class of molecular level simulations.

For chemical reactions, we have found that simply placing structures of the molecules above their occurrence in the chemical reaction has little effect on learning (*4*). What is more powerful is showing the effects of a chemical reaction on a collection of molecules. Such visualization emphasizes that chemical reactions are rules that are applied to collections of molecules. Figure 7 illustrates the "extent of reaction" coordinate generated by applying the reaction rule (2 NO_2 react to make 1 N_2O_4) to a collection of initial NO_2 molecules. This coordinate is central to understanding key concepts in chemical equilibrium. For instance, shifting of a reaction towards reactants or products is occurring along this coordinate, which is invisible in the original reaction equation to which this idea is usually attached. Think-aloud interviews with students solving equilibrium problems revealed substantial confusion regarding this coordinate. For instance, students could not correctly state the distinction between Q and K, and made errors related to a failure to distinguish initial from equilibrium conditions. This coordinate is held so innately by instructors that they fail to emphasize it in their instruction, yet our studies suggest that lack of flexibility with this concept is one of the factors limiting performance in equilibrium problem solving (*2*). Molecular visualization is a powerful means for teaching this concept which, while not difficult, does need to be made explicit and highlighted as central to reasoning about chemical equilibrium systems.

The other key innovation in our equilibrium course is the introduction of a single unifying strategy for solving equilibrium problems that involve reactions with large or small equilibrium constants, K, such as commonly occurs in acid-base and solubility equilibria. The first step in this strategy is to run all strong ($K>>1$) reactions occurring in the system to completion, via limiting-reagent style computations. This first step determines the concentration of all majority species, i.e. those with large concentrations. Since the equilibrium constants are large, but sill still finite, those species that act as limiting reagents in the first step have small but non-zero concentrations. The relation $K=Q$ at equilibrium is used to determine the concentrations of these minority species. This majority-minority species strategy has the advantage of providing a single strategy for all equilibrium problem solving. This strategy also focuses student attention on the chemistry occurring in the solution by beginning the computation with the identification of strong ($K>>1$) reactions. However, given the large difference in majority and minority species concentrations, it is difficult to use molecular-level visualization to teach this aspect of the material.

The next session discusses our CIMS project, in which molecular level visualization plays a central role in the instruction.

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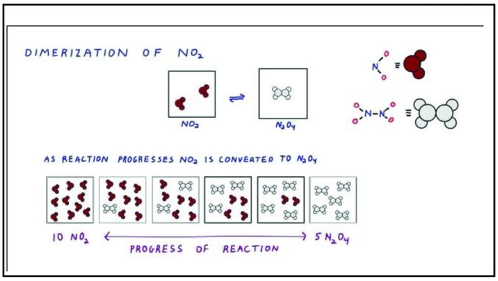

Figure 7. Progress of reaction illustration.

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Some Design Principles

In this section, we consider how our past experiences have informed the design of our most recent curriculum development project: Core Ideas in Molecular Science (CIMS). After briefly summarizing the educational motivation and goals of the CIMS project, we will discuss the design of this project in the context of some general design guidelines.

The goal of CIMS is to develop interdisciplinary instructional materials that are appropriate for use in discipline-specific courses, yet designed to help students draw connections across multiple disciplines. As advances in science and engineering continue to accelerate, so does the amount of knowledge needed to become proficient in a technical domain. The blurring of lines between domains further increases these knowledge requirements (*27*). As biology becomes increasingly molecular, biologists must become increasingly proficient at chemistry. As chemistry becomes increasingly hyphenated into biological-, materials-, and environmental- chemistry, chemists must couple their knowledge with that of other domains. As physics widens to accommodate novel systems inspired by biology and engineering, physicists are embracing interdisciplinary points of view, such as is seen in soft condensed matter. As the scope of materials science continues to expand beyond its roots in metallurgy and ceramics, engineers must master ever broadening bases of knowledge, including the molecular science needed for soft and nano materials. Our goal is to develop resources that help address the educational challenges posed by these recent advances in the sciences.

Match the Modality to the Context of Use

In the above discussion, the modality of educational components was somewhat narrowly discussed in terms of moving explanation and practice online. The utility of such changes in modality, however, relates to a broader issue of the context of use. Moving explanation online is useful if it makes the explanations more readily available to students and allows better pacing. Moving practice online is useful if it encourages students to engage in more regular and evenly spaced practice. In our past projects, the educational context of introductory college classes has informed the modality of the content. Our virtual lab activities are packaged as online homework, since graded homework assignments are easy

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for instructors to adopt and so provide a convenient entry point to these courses. Our stoichiometry materials target students who may need to brush up on this important foundation material, and so are packaged as stand alone tutorials that combine explanation with practice. Our equilibrium materials correspond to a new instructional approach and so are also a complete enactment of instruction.

Our modality choices for the CIMS project are influenced by our goal of helping students see connections between the uses of molecular science in various domains. Ideally, making these connections explicit will lower the burden on students by taking a large volume of educational content from various courses and helping students learn the material as a single coherent set of knowledge. We are therefore designing materials for use in current discipline-specific courses and are covering existing topics in these courses. By working within existing course topics, we may avoid contributing to one of the problems we are trying to address, that of the increasing burden on students due to the growing topic lists in these courses. To provide coherent instruction on molecular science across these disciplines, we need to alter the nature of both the explanation and practice. Nevertheless, our target is college classes and so our entry point is through assigned online homework. We are therefore creating materials that can be assigned as homework in the target courses, but unlike our virtual lab homework, these materials combine explanation with practice. We are creating different versions for each of the target disciplines that share the key features of the explanations and use the same visualization and simulations tools but that tie the ideas to different systems or applications. For instance, our materials on reaction energy diagrams and free energies used a single set of core explanations and simulations, but applied these to reactions between small molecules for chemistry and protein folding for biology.

Take the Time To Analyze and Re-Envision the Domain

Changes in modality can bring considerable educational benefits, and matching modality to the context of use is essential for materials to be useful in practice. However, the greatest benefits to learning are likely to come from fundamental changes in the nature of the explanation or practice. Such fundamental changes arise only from a careful analysis of the domain from a broad range of perspectives, which takes time and effort. The domain analysis should also be informed by student feedback and data. Our virtual lab activities are driven by the desire to help students draw connections between their paper-and-pencil calculations and actual chemical systems. To do this, the virtual lab implements a new mode of practice that encourages such connections. Our equilibrium module is based on extensive analysis of the domain, which identified important aspects of the knowledge that are left implicit in traditional instruction. The module implements a new mode of instruction that makes this tacit knowledge explicit.

In the CIMS project, we set up a process for identifying and analyzing instructional targets in a systematic manner. We also encourage a sufficiently open discussion among representatives of the different disciplines that the process is open to fundamental changes in instruction or practice when appropriate. Our overall strategy is to identify the *recurring patterns* that experts use to organize their knowledge and develop educational materials that make these patterns explicit to students. Our approach involves regular design meetings of materials scientists, chemists and biologists to identify patterns of thought that recur across these disciplines. Experts are able to apply knowledge across disciplines because they identify and use these recurring patterns. However, analysis of current discipline-specific instruction reveals that students are given little support or practice in identifying and capitalizing on these ways of thinking. Interdisciplinary connections are typically presented implicitly and often quite late in a scientist's or engineer's career. Our goal is to create materials for discipline-specific courses that provide students with explicit, coherent frameworks that draw connections across domains. In selecting targets for our instruction, we analyze the content of the target courses to identify concepts and conceptual frameworks that are:

- **Central to each of the domains** such that we do not divert instructional time to topical areas that instructors will view as peripheral to their course
- **Have strong leverage** such that improved mastery of the material will substantially enhance students' ability to engage with core ideas within and between the domains
- **Difficult to teach and learn** such that the development focuses on areas where improved instruction will be of most value

This process has led to a number of candidate topics for interdisciplinary instruction. Experts from each of the domains could readily identify with the ideas as being core to their thinking, could cite specific instantiations of the ideas both in their course and in their research, and could recall (both from their personal experience and interactions with students) that drawing connections between the occurrence of these ideas in different domains involves considerable effort. Post reflection revealed that the overlaps identified between these domains all lie within the area of molecular science, defined here as "understanding how molecular structure and motion lead to emergent macroscopic properties", and "developing methods to build desirable molecular structures".

The first recurring pattern we indentified was that of "reaction paths and energy landscapes". The design effort then shifted to a detailed cognitive analysis of the content, to identify what specific knowledge must be learned and practiced to be flexible with this pattern.

Continued discussion has led to three more recurring patterns, or core ideas, that are our current development targets: "economies of exchange" which draws connections between proton, electron and other types of exchange equilibria systems; "weak versus strong forces" which connects the magnitudes of covalent and intermolecular forces to emergent macroscopic properties and self-assembled structures; and "thermodynamic versus kinetic control" which considers how man-made and natural systems direct formation of desired products. These remaining core ideas share a common simulation and visualization framework, which is discussed in the next section.

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Use Configurable Simulation/Visualization Components That Target the Correct Interaction

Reflections on our past design of educational software components reveals two general guidelines or strategies. The first is the use of configurable components, as discussed above, to allow educators without programming expertise to author and modify activities. The second is placing the student interaction and manipulatives at the location of difficulty. In the virtual lab, the targeted difficulty is drawing connections between paper-and-pencil activities and actual chemistry, and the software targets this by engaging students in the design and interpretation of experiments.

For the CIMS module on reaction paths and energy landscape, the educational goal is helping students understand the meaning and power of diagrams of the type shown in Figure 8. The difficulty relates to the level of abstraction in such diagrams, with the meaning of both the x and y axes drawing on large sets of previous knowledge, and the need to consider temperature (which is invisible in the diagram) when drawing conclusions. The instructional sequence uses visualization and simulation tools to systematically unpack these dimensions. [http://matdl.org/virtuallabs/index.php/CMU09106_VirtualLab].

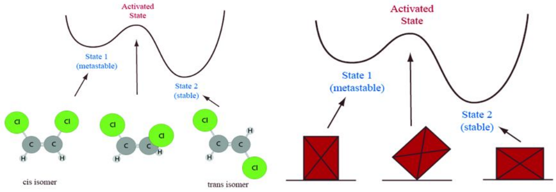
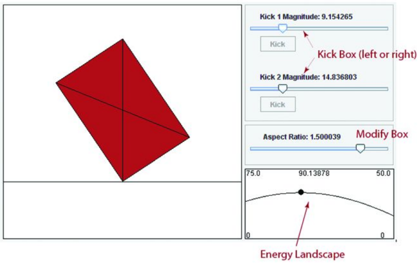


Figure 8. Analogy between chemical and physical models.



Kick 1 Magnitude: 9.154265

Kick 2 Magnitude: 14.836803

Aspect Ratio: 1.500039

90.13878

Kick Box (left or right)

Modify Box

Energy Landscape

Figure 9. Simulation to support meaning of energy landscapes

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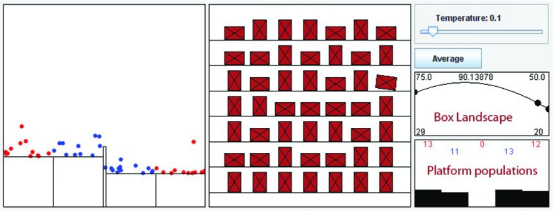

Figure 10. Final simulation in sequence showing population distributions resulting from constant temperature dynamics. Students are prompted to connect the various models and representations.

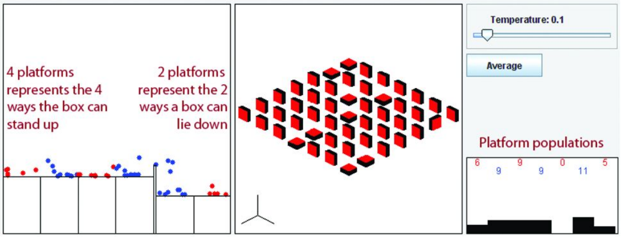
4 platforms represents the 4 ways the box can stand up
2 platforms represent the 2 ways a box can lie down
Temperature: 0.1
Average
Platform populations
6
9
9
9
0
11
5

Figure 11. Use of a 3-D box to illustrate entropy and free energy.

To ground the energy landscape in the physical world, Don Sadoway's lectures at MIT use the box analogy of Figure 8. This analogy formed the basis for a simulation (Figure 9) in which students explore connections between the shape of a box and the energy landscape corresponding to tipping the box over. A principle mode of instruction is having students draw connections between the various representations. Here, the student activities connect the dimensions of the box (left panel of Figure 9) to the energy landscape (right panel of Figure 9) and to molecular isomerization (Figure 8).

Experts are quite flexible in drawing connections between energy landscapes and emergent properties such as the rate of a chemical process and the equilibrium distribution between various minima. The conceptualizations needed to draw these connections are entirely missing from the energy landscape diagrams themselves (the expert notation). To remedy this, a series of representations are used to make these connections more explicit. These simulations show balls (and/or boxes) on a vibrating surface that represents the random thermal motion of a heat bath. The simulations slowly add features and representations, culminating in the simulation of Figure 10. As the temperature is increased, the average height of the balls bouncing on the platform increases, as do the number of boxes being kicked up to stand on their short side. The instructional materials guide students as they explore the effects of simulation parameters such as temperature on the distributions of balls between the upper and lower platforms (or boxes between the standing up and lying down configurations). Students are also prompted to draw connections between the various representations. The materials also provide explanations and practice with key underlying concepts including the Boltzmann distribution, the relation between barrier height and reaction rate, and the relation between thermodynamic driving force and the equilibrium distribution.

Finally, the simulation in Figure 11 uses a three-dimensional box to introduce the distinction between energy and free energy (a refinement on the meaning of the y-axis). The box has four sides on which it can stand up (in a meta-stable state) and two sides on which it can lie down (in a stable state). The relative number of ways to stand up versus lie down is represented in the platform simulation as four high-energy platforms and two low-energy platforms. This differing number of configurations (4 vs. 2) is used to illustrate the microscopic meaning of entropy (the higher-energy state has larger entropy since there are twice as many ways to stand up as lie down). The instructional materials use this system to illustrate the meaning of an entropy-driven process. At sufficiently high temperature, the average height of the bouncing balls is bigger than the energy difference between platforms, and the result is that the total number of balls on the higher-energy platforms is greater than the total number on the lower-energy platforms. The population in the higher-energy state is greater, simply because there are more high-energy platforms. The transfer of most of the population to the higher-energy platforms at high temperature is an example of an entropy-driven process. Connections are then drawn to important entropy-driven processes such as the unfolding/denaturing of a protein (biology), desorption from a surface (materials science), and the breaking of a chemical bond (chemistry).

The remaining three core ideas targeted by CIMS relate to the connection between molecular interactions and macroscopic outcomes. In “economies of exchange”, the connection is between relative binding energies for a proton or electron to different species, and the resulting concentrations of these different species. This is then related to macroscopic properties (pH and redox potential) and phenomena (buffering). In “weak versus strong forces”, the connection is between the magnitudes of the molecular-level forces and macroscopic properties (melting and boiling points) and phenomena (self-assembly). In “thermodynamic versus kinetic control”, the connection is between molecular structure and forces and the formation of kinetically-favored versus thermodynamically-favored products.

The location of difficulty for each of these topics is connecting the atomic-level interactions to the macroscopic outcomes. The set of simulation tools we are developing allows students to modify the rules of these interactions and explore the consequences on a large ensemble of molecules. Rather than using molecular dynamics (which integrates Newton’s laws), we are designing a rule based system. For instance, consider a simulation showing competitive binding of an analyte molecule to two different proteins, as related to the core idea of “economies of exchange”. Our goal is to show how the relative free energies of binding and the temperature interact to determine the equilibrium distributions, and to build from this to concepts such as the role of dynamic equilibrium in protein mediated transport across a membrane. In molecular dynamics, one would need to create force laws that lead to the desired behaviors. We are instead implementing a rule based system, where decisions such as whether a protein and analyte bind are made based on rules. In this case, the rule compares a random number to $\exp(-\Delta G/RT)$ to determine if the two components bind on a collision. Our goal is

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to develop a general tool that allows users to set rules and explore the consequences of these rules on the simulation's emergent behavior. Student practice that involves changing the rules to achieve a certain macroscopic outcome will give students direct practice with connecting atomic level interactions to macroscopic outcomes.

Remain Flexible with Technology Choice

A challenge to development of online content is the continuing evolution of the technical environment. The relative popularity, and therefore level of support, for various technical platforms waxes and wanes over time in ways that are difficult to predict. As a result, the choice of platform is necessarily based on incomplete information on the future potential of these platforms. In choosing a platform, we aim to be sufficiently conservative that we do not jump onto technologies that are exciting but transitory or not yet well-enough developed. On the other hand, we want to be sufficiently flexible that we do not become entrenched in a given approach and miss out on technologies that could substantially reduce the development effort or enhance reuseability. Fortunately, as technology evolves and becomes more powerful, the development of interactive content becomes easier.

While choice of platform is always fraught with uncertainty, the following three attributes of a good technical platform can help to guide the decision. The first is ease of access for the end user. This is important because prior experience suggests that requiring users to install additional Web plug-ins, or otherwise take steps not directly related to the educational interaction, can reduce the number of users. The second is ease of development, which speaks in favor of well-established, mature platforms because these typically offer good authoring tools, abundant documentation, and a wealth of code libraries. The third is ease of reuse and maintenance of developed content, which is enhanced by systems that allow the user interaction to be customized without requiring programming expertise.

We set the above technical platform attributes as goals when beginning development on all of the projects described above. However, because these projects began at different times and with different needs and objectives, the precise platform we chose is not identical across all of our projects. For example, our virtual lab was written in JAVA, which is a full language rivaling C++ and so has sufficient power to implement almost any form of interaction. But this power comes at the cost of more complex development which can slow development and hinder reuse. The CIMS development began with Java because we had considerable experience with this platform and we thought that implementing molecular dynamics would require the power of a full programming environment. In addition, we wanted to stay with an open technology that would allow others to modify the simulations without purchasing proprietary development tools. However, as the project evolved, we realized that graphic designers were now able to implement quite complex particle-based animations in the Adobe Flash platform. In particular, the Flint Particles system [http://www.flintparticles.org] provides an open source, stable code base for handling the motion of thousands of particles in real time. This system was built to allow graphics designers to create advanced visual effects, however, the approach could be extended to implement

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the rule-based molecular dynamics needed for CIMS. Furthermore, the Flash platform had evolved to include a suite of development tools and approaches, including Flash Builder, which is freely available to academic institutions and students. This lowers the economic barriers to promoting reuse. In addition, Flash Builder and Flint Particles use the Flex software development kit to help separate the design of the user interface from the development of simulation codes. While development of the simulation code requires considerable expertise, the use of Flex to create applications from the simulation code is less complex and so may be accessible to a larger proportion of users. Finally, although the Web browser plug-ins necessary to run Java and Flash both have a substantial installed base, the installed base of Java is in decline, while that of Flash is near 100% of Internet-connected computers. The widespread use of Flash in commercial Web sites, Internet video, and interactive games suggests that it is likely to be well-supported for the foreseeable future.

As noted above, we began work on CIMS using Java, but switched to Flash along the way. This switch came at the cost of learning a fairly complex set of new development tools. However, the decision was based on considerable research into the various alternatives and was decided upon when it appeared that the long-term benefits would outweigh the short-term costs. However, only time will tell if this decision pays off.

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Closing Comments

This chapter explores a variety of issues related to the design of educational components that can be repurposed to different educational contexts and that can be iteratively improved by a community of educational practice. The underlying goal is to enable digital libraries to support open and collaborative design of chemistry instruction. Such collaboration has the potential to go beyond modality changes, which move traditional forms of explanation and practice online, to more fundamental changes in the nature of the explanation and practice. In our work, such fundamental changes have been linked to our evolving understanding of the student as learner and have allowed us to target a variety of instructional approaches more precisely. Our virtual lab targets the connection between paper-and-pencil computations and laboratory chemistry. Our equilibrium module targets knowledge that is important for understanding the domain but is left implicit in current instruction. Our CIMS project targets those components of chemistry that are important across several domains, with the goal of providing students with a more coherent understanding of molecular science.

As we look to the future, we imagine both expansion and refinement of these efforts. Expansion is expected and encouraged along two fronts. The first front for expansion is to engage more members of the community in the development and refinement of the instruction. Digital libraries enable this by allowing instructors to assemble components in various ways, and to use classroom experience to determine what works, what does not work, what components can be improved, and what topic areas should be most focused on for future development. To support such community input, components must allow authoring of interactive content to be done in as easy a manner as possible. The second front for expansion is that of topics, with more areas of chemistry becoming the target for thoughtful instruction.

In addition to expansion, refinement is expected as we both become more aware of what it is that students find challenging and how technology can be used to help students address such challenges. As new explanations and modes of practice are developed, the experience gained from watching students interact with this content will continue to expand our understanding of how students learn. For instance, the comparison described above, of students solving paper-and-pencil problems versus virtual lab activities, revealed that students use means-ends analyses to solve paper-and-pencil problems in a shallow manner that does not give sufficient practice with the deeper chemistry knowledge. Given this insight into student learning, one can design practice that gets at the deeper knowledge. Another area of refinement is becoming more precise about selecting concepts and skills that have the greatest payoff for the learner when learned well and deeply. For instance, the CIMS project has a process for selecting topics in molecular science that have power in multiple domains.

Such expansion and refinement in digital library efforts for chemical education has the potential to substantially improve teaching and learning in chemistry.

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Chapter 14

Developing ChemPRIME: Transforming the Didactics and Pedagogy of the General Chemistry Course with a Wiki Text

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ChemPRIME (Chemical Principles through Integrated Multiple Exemplars) is a wiki text, so it offers several advantages due to the wiki medium. But the format in itself isn't a reason to use an educational strategy. The ChemPRIME wiki text takes advantage of the medium to offer didactic and pedagogical advantages that could not be realized through any other format. There will undoubtedly be many wiki texts, and several have appeared already. Many will amount to little more than online versions of printed texts, taking little advantage of the medium except perhaps by adding a few hyperlinks. The appeal of "open textbooks" in the current textbook market cannot be ignored, and the Creative Commons licensing in itself makes wiki texts appealing. But Web published materials are not always trustworthy, nor do they make unique contributions, or exploit transformative approaches enabled by the Web. While the ChemPRIME wiki is in its infancy, a structure has been created that allows a novel approach to teaching general chemistry.

Toward a New Didactics of Chemistry

A visitor to the Chemical Heritage Foundation in Philadelphia (or non-chemist reader of ***Chemical & Engineering News***) might wonder what chemistry is really about. There are exhibits of living plants, of minerals, of engineering and artistic creations. What do they have in common? Nothing, ostensibly. What they share is the way the exhibits are interpreted or explained in the accompanying textual labels. Chemists have known, but have not proclaimed outright, that chemistry

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

does not reside in the *subject* of our study, but in the kind of *explanation* that we offer for its properties and behavior (*1*). Chemistry is in the mind of the beholder; it is the discipline that explains, or understands, *anything and everything* in terms of the properties of atoms and molecules (*2*). The Slogan of the American Chemical Society is "Chemistry for Life", which implies that chemistry can add a dimension to every aspect of modern life.

Educators repeat the mantra "Chemistry is the Central Science." It's time to prove it. Proving it requires a change in chemistry didactics. While pedagogy deals with interpreting the teaching content to students, we take didactics to involve development of the teaching content of a discipline to reflect the activities of its practitioners. The distinction we make between didactics, (dealing with teaching and creating the body of knowledge that is taught), and pedagogy (dealing with how students learn) is not always made in this way (*3*), and the two terms are frequently conflated, but the distinction is a useful one. When a new discipline emerges, part of what makes it recognizable as a discipline is an agreed-upon body of work that is taken as paradigmatic, and which is used to train new practitioners. Similarly, when an established discipline, like chemistry, undergoes significant changes in practice, that change should be reflected in how the discipline is taught, that is, in its didactics.

Practitioners of chemistry are increasingly dispersed in academic departments dedicated to a variety of subjects. This trend started some time ago. In his Priestley Medal address in 1991 Harry Gray predicted the end of chemistry departments because chemistry would be taken up by other fields until the only part left to "pure chemists" would be organic synthesis. The Committee on Challenges for the Chemical Sciences in the 21st Century of the National Research Council (*4*) reported that, "Chemistry and chemical engineering have changed significantly in the last decade. They have broadened their scope into biology, nanotechnology, materials science, computation, and advanced methods of process systems engineering and control so much that the programs in most chemistry and chemical engineering departments now barely resemble the classical notion of chemistry. We conclude that chemists and chemical engineers must put much more effort into effective communication with the media, and with students from kindergarten up. We also urge that our profession make much more effort to attract women and minorities."

Chemists like to suggest that "everything is a chemical" because they claim that everything *can* be understood in terms of its constituent atoms and molecules. But that acknowledgment seems to imply that chemistry must be dispersed among other disciplines which are defined by their subject matter. If we claim that everything is a chemical, shouldn't we show chemistry students from all disciplines how that's true in each of their disciplines? Can that be done without an impossibly large text?

ChemPRIME reflects the changing nature of the discipline of chemistry with a new didactical approach, while incorporating several pedagogical advantages, both made possible by the wiki format.

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The Structure of ChemPRIME

ChemPRIME reflects the evolution of the chemical sciences toward truly being a central science, contributing to understanding in many subject areas, like the Chemical Heritage Foundation displays. Each chapter section in ChemPRIME presents a menu of applications of chemical principles to a variety of subjects. The menu includes "CoreChem", a standard textbook presentation (*5*) that is now an editable wiki text, and additional "Tracks", which include Geology, Physics & Astronomy, Everyday Life, Foods, Sports, Biology, Culture, Environment, Forensics, and Lecture Demonstrations. The Tracks run throughout the wiki text, and will gradually be populated with "Exemplars". Exemplars are applications of the CoreChem concepts to interesting problems in each of the fields. The Tracks will take time and user participation to populate with Exemplars, and our hope is that instructors and students will contribute their favorite applications of chemistry. For example, since many of the students in the General Chemistry course are Biology majors, we've developed mostly Exemplars in the BiologyTrack. In principle, it would be possible for a student to learn all the concepts in the course by following the Biology (or any other) Track, or a student could change from Track to Track, as interests change. The Exemplars are designed to have the same incoming prerequisite knowledge, and outgoing skills as CoreChem for each topic, so the concepts that students learn will be the same, while the applications vary.

Exemplars are not difficult to conceive for most of the concepts taught in General Chemistry; if they were, it might suggest that those topics *do* lack relevance and interest. Exemplars are like the "boxed applications" now found in some texts, or the case study approaches favored by some teachers, but their arrangement in ChemPRIME presents unique advantages, as explained below. Exemplars are incredibly interesting and enjoyable to write. They can renew an instructor's interest in the course.

Some sections of ChemPRIME already have Tracks populated with a number of Exemplars. For example, the ChemPRIME section on *Enthalpies of Fusion and Vaporization* (*6*) includes the following:

In the Foods Track, an Exemplar called "The Amazing Ice Diet", explores the caloric demand of melting ingested ice, and the plausibility of the claim that one could lose weight by eating ice or drinking cold water. To lose a significant amount of weight takes a lot of ice, of course; melting a few hundred grams would only amount to a percent or so of our daily caloric requirement. But the energy isn't insignificant, and outdoor survivalists warn against eating too much snow when lost in the woods with no food or water.

The History/Culture Track has an Exemplar called "Joseph Black and the Melting of Ice" where Black's own description of his famous "gedankenversuch" is presented. It describes the catastrophic effects that the Spring ice melt would have if the heat required were so minuscule as " to be discoverable by the application of a thermometer". Figure 1 shows an historic ice calorimeter from the ChemPRIME Exemplar.

Another Exemplar in the Culture Track is called "Ice Houses" and asks "What do these three, culturally diverse buildings have in common?" Two of the figures are shown here (Figures 2 and 3). They are pictures of an icehouse ("ghiacciaie") in Boboli Gardens, Florence and a middle ages icehouse ("yakhchal") in Kerman, Iran, respectively.

The chemistry content deals with the modern equivalent in electrical energy needed to produce the amount of ice in a typical ice house, and thus examines the economics of storing ice. Although refrigerators are still occasionally called "ice boxes", students may be surprised that the real thing was used extensively in the U.S. in the last century, when icehouses were common.

The Everyday Life Track has an Exemplar entitled "Why are Air Conditioners Rated in 'Tons' of Cooling Capacity?" which explains that a ton of thermal capacity is the latent heat of a ton of ice (just over 1 m^3) released in 24 hours. Figure 4 from the Exemplar shows an early American ice house. In modern terms this one ton of cooling or heating capacity is 12,000 BTU/hr (over 300 MJ/day), possibly enough to cool a typical modern house.

The Biology Track includes an exemplar called "Protecting Citrus Trees from Freezing with Freezing Water", illustrated with Figure 5, which shows cankers caused by Pseudomonas syringae, a bacterium which contains "ina" (ice nucleation active) genes. Plants infected with that bacterium are much more likely to suffer frost damage, because it catalyzes nucleation of ice at the freezing point. This suggests other Exemplars dealing with the nucleation mechanism in kinetics, as well as the efficacy of an "ice minus" bacterium, lacking the ice nucleation protein, which has been developed by recombinant techniques.

The Environmental Track discusses Domestic Energy Storage in Phase Change Materials (PCMs), and uses Glauber's salt as an example. Intermittent power sources like solar and wind may use a variety of chemical storage systems, including fused salts, which are interesting to investigate and could be the basis for additional Exemplars.

The Geology Track has an Exemplar dealing with heat of fusion of Magma in "plutons" (Figure 6) and the implications for young earth creationism. The cooling rate for the Earth was used by William Thompson in the nineteenth century (before radioactive heating was known) to estimate the age of the Earth at between 20 and 400 million years, while young earth creationists claim an age of around 6000 years. Plutons are intrusive igneous rock crystallized from magma, and we know that plutons like the Palisades Sill along the western Hudson River in New York and New Jersey would take at least 2000 years to solidify, and longer than 10,000 years to cool to ambient. The phase change contributes a significant amount to the age prediction. Of course, radioactive heating, which confounded thermometric predictions of the Earth's age, also provided a better way of measuring it.

We use bomb suits (Figure 7) as an exemplar for enthalpies of phase changes in the Physiology/Sports Track. Bomb suits are particularly interesting, because they use fusion in ice packs, which are part of the suits, to remove the heat that evaporation of water from the skin would otherwise remove. Thus the latent energies associated with two phase changes can be compared.

Finally, the Physics/Astronomy Track features an Exemplar about "*virga*", precipitation that evaporates before it reaches the ground (Figure 8). Virga apparently occurs on Mars as well as Earth, but on Mars, it is more likely to be snow or ice that sublimes in the atmosphere as it falls. Since the discovery of

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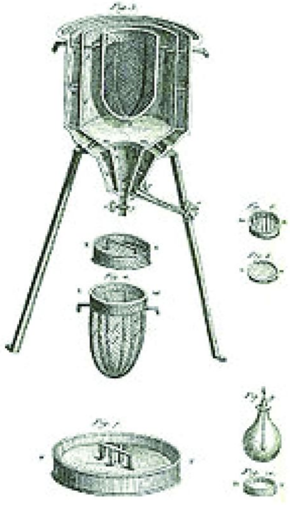

Figure 1. The original ice-calorimeter, used by Antoine Lavoisier and Pierre-Simon Laplace in 1782-83, to investigate Joseph Black's prior discovery of latent heat (reproduced from reference (51)).

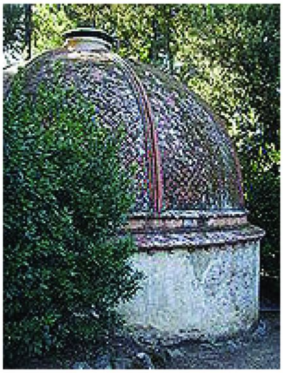

Figure 2. A ghiacciaie in Florence, Italy (reproduced from reference (52)).

water on Mars, a lot of information is available about the fusion or sublimation of ice deposits on the planet. Because the temperature, pressure, and composition of the atmosphere differ from those on Earth, phase changes of water on Mars may provide some interesting educational opportunities.

A second set of Exemplars that illustrates the possibilities we envision appears in the ChemPRIME section on *Density* (*7*). Here the Culture Track has an Exemplar called "The Platinum Flute" which links to a performance of "Density 21.5", a composition by Edgar Varese for the inaugural performance of a platinum (density = 21.5 g/cm^3) flute. Normally, we might not use a piece of music as the basis for an Exemplar just because it has a relevant sounding title, but Edgard Varese was one of several composers who were influenced by science (his "Ionization" is an excellent musical interpretation of the quantized atomic

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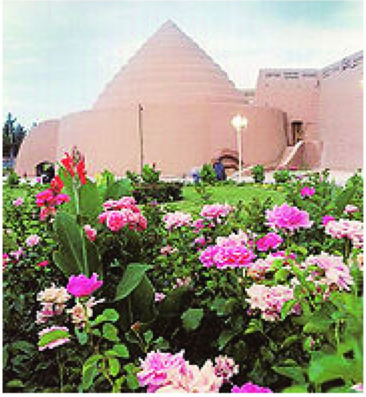

Figure 3. A middle ages yakhchal in Kerman, Iran (reproduced from reference (53)).

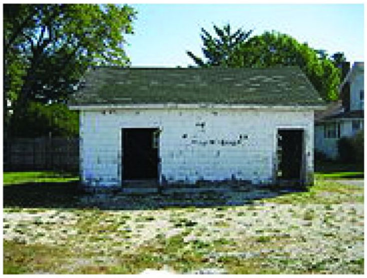

Figure 4. An Early American Ice house at a Texaco Gas Station on Historic Route 66 (reproduced from reference (54)).

processes). Some popular songs do provide content ("Entropy" by Moxy Fruvis comes to mind). They are easy to find with iTunes®. Other Exemplars in the Density subchapter deal with the density of black holes in the Physics/Astronomy Track; lava lamps in the Everyday Products Track; density of LDLs (low density lipoproteins) in the Biological Track; bulk density of soils in the GeologyTrack; and density sorting of recyclables in the Environmental Track. In the Sports Track, the "Floating Footballs" Exemplar discusses the myth that footballs filled with helium can be kicked farther than those filled with air. It's easy to link to sources of background information (the source of the myth is Ray Guy, punter for the Oakland Raiders from 1973-86), and to videos like the "Mythbusters"® episode where the myth was investigated.

The Educational Philosophy behind ChemPRIME

ChemPRIME has been designed to resolve a conflict between two philosophies of teaching chemistry: Many teachers are convinced by pedagogical arguments that it is preferable to present chemistry as a logically developed, hierarchical structure of knowledge, where each idea depends on previously

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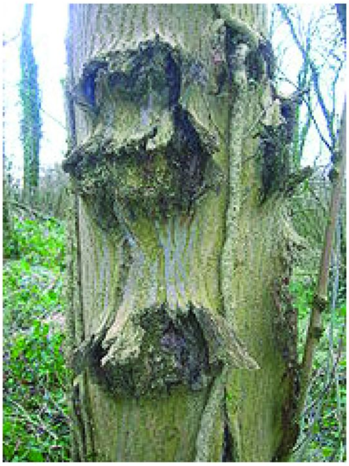

Figure 5. Ash canker caused by Pseudomonas syringae, which is responsible for frost damage (reproduced from reference (55)).

Figure 6. Magma which solidifies to "plutons", whose cooling rate can be used to set lower limits on the age of the Earth (reproduced from reference (56)).

developed concepts and is prerequisite for subsequent ideas. But students prefer "top down" approaches, introducing concepts through higher level, interesting examples. There are good pedagogical reasons for this as well (*8*). Teachers have responded with various "case study" approaches, where the theoretical background needed to understand the case is provided on an "as needed" basis for explaining some (presumably interesting) case. While this provides a context that may motivate students who happen to be interested in that particular case, teachers are generally uncomfortable with the disorganized presentation of theory, and any student who is not interested in the case at hand gains no inspiration through the case study approach.

But why choose? ChemPRIME gleans the best of both approaches: it presents the theory in a logically developed manner, but for every theoretical concept, it presents a selection of exemplars from different subject areas, so students can learn the theory in the context of a subject that interests them.

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Figure 7. Bomb suits use ice for coolant because they prevent thermoregulation by evaporation of perspiration (reproduced from reference (57)).

Figure 8. Virga falling from a nimbostratus cloud on Earth may be analogous to snow virga on Mars (reproduced from reference (58)).

Toward an Improved Curriculum

ChemPRIME responds to several of the trends for reform of General Chemistry that are commonly recognized (*9*), and addressed with growing urgency. Much of the concern seems to be with the didactics of chemistry; that is, with the body of chemical knowledge that is appropriate to teach, and the manner in which the discipline is presented in chemistry courses. For example, it is often suggested that General Chemistry courses are directed toward chemistry majors (a minor constituency) while they ignore the needs of others. We have no excuse for doing this, given the current state of the discipline. It also said that we often fail to engage student interest (a problem that may be didactical or pedagogical), that we cover too much material, and often fail to incorporate proven pedagogical principles.

ChemPRIME addresses the first concern directly by providing exemplars from different fields. Modern general chemistry texts are incredibly rich compared to those of decades past. Most teachers expect the “boxed features” found in modern texts to motivate students. The features are generally excellent, but since there is usually only one or two per chapter, they may match the interests of only a fraction of readers. A wonderful application of chemistry in medicine may fascinate some students, but may be as “irrelevant” as the bare-bones chemistry to others. The ChemPRIME approach directly addresses this problem by providing a menu of applications for every major concept in the course, so a student may (when ChemPRIME is fully developed) take the entire course in one track that suits his interests, or switch from track to track for a smorgasbord of chemistry applications.

If we accept as realistic the claim that chemistry must be relevant to the needs of students in a variety of disciplines, ChemPRIME provides a means of measuring how effective we are in doing so. If it is difficult to come up with an exemplar for a topic in the General Chemistry curriculum for the Geology, Engineering, or Biology tracks, perhaps we should reconsider the value of that topic. We decide to retain it in the liberal arts tradition that some things are simply worth knowing “for their own sake” in the interest of a well-rounded education, but at least that decision will be explicit. And if we do find relevant Exemplars for each of our topics, we’ve proven the criticism wrong and must look for other reasons for student failure. Relevancy may be necessary, but it isn’t sufficient, to engage students (See below).

Finally, there is concern that General Chemistry texts are too long. While printed texts typically achieve relevancy they can claim by adding “boxed features”, in ChemPRIME, students read any chosen Exemplar *instead* of the “CoreChem” text. ChemPRIME integrates the Exemplars, so that each one has the same prerequisite knowledge and learning outcomes, which are standardized for each section. The CoreChem Track is fairly terse and presents just the essentials, and most Exemplars are of similar length. While the entire wiki text may be virtually unlimited in size, the pathway that any particular student takes through it may be short and concise, presenting only information relevant to the student’s interest, but covering all the concepts of the General Chemistry course.

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“Open Books”, eBooks, and The “Broken Market” of Textbooks

Textbooks have grown in price as well as size as a result of practices that have attracted the attention of the U.S. Congress, the Government Accounting Office, the U.S. Public Interest Research Group (PIRG), student aid groups, and state governments. Availability of print texts, open source, and commercial Web texts could provide the perfect mix of approaches to satisfy any teaching or learning style, but the textbook market is subject to unusual pressures which don’t always work in students’ or their professors’ favor.

The term "Broken Market" was used by economist and former president of Old Dominion University James Koch to describe the textbook market (*10*). The analysis was commissioned by the Advisory Committee on Student Financial Assistance (ACSFA) because the cost of texts may, sadly, have an impact on student access to education. Koch pointed out that, unlike other consumer items, textbooks are not selected by the users (students), but by professors, who then require them in courses. A “broken market” results because ordinary market checks and balances cannot operate. It’s easy to sympathize with students who

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balk at purchasing a text for well over $100, compared to books on the best-sellers list for $25, especially when texts often differ by less than the options choices most new car models. As a result, substantial percentages of students do not buy textbooks (*11*). Koch's essay provides many interesting insights into the text publishing industry from an economist's point of view. He notes the similarity of the textbook industry to the medical care market, where prices rise because insurance companies, not the care receiver, pay for the care.

The cost of textbooks has attracted the attention of the Government Accountability Office which found (*12*) that the cost of textbooks increased at twice the rate of inflation between 1986 and 2004, and can cost 72% of the total cost of tuition and fees at public two-year colleges. On 8/14/2008, then President Bush signed the Higher Education bill (H.R. 4137) which passed Congress by large margins. Starting next year, it requires publishers to sell ancillary items like CDs separately from textbooks, and requires publishers to divulge book prices to professors considering adoption, although it refrained from more direct price controls (*13*).

In response to these pressures, publishers have begun producing "*Open Source Textbooks"* and *Electronic Textbooks*. At least one major publisher, Flat World Knowledge (*14*), publishes free, online, college textbooks. Profits result from sales of soft cover editions, audiobooks, and ancillary materials like study guides. The books may be created or edited by the instructors who use them, so in a *limited sense* they are open source texts, but they retain a more or less standard copyright and usage control. Some electronic books are offered online for free, for example from academic sites like the MIT OpenCourseWare initiative (*15*). No chemistry open source textbooks appear to be available at these sites, and none is listed on the Student PIRG (part of the US PIRG coalition) site (*16*). It appears that there is a market for a truly open source General Chemistry text, especially one built on the wiki model where all of the content is under a Creative Commons license.

Several chemistry texts are now available online, although they are not wiki texts or editable by users (*17*). At Harvard, Professor James G. Anderson provides the textbook he wrote for a non-major's course, Physical Sciences 1: "Chemical Bonding, Energy, and Reactivity," for free, through the course's Web site. He says "I see it as a win-win-win. For students, for the environment, and for the teaching staff" according to the Harvard Crimson (*18*). The profit incentive for both publishers and authors has led to the production of many high quality books, which they say, justifies the cost. It also allows authors to dedicate time, beyond that supported by universities, to development of quality course materials. The Crimson article cited above reports that another professor requires his own commercial book for the college's introductory economics class of 2,278 students, saying "I don't talk about personal finances." Some faculty donate their earnings, (sometimes by policy (*19*)) but the high text cost and lingering ethical issues make one wonder if open- or wiki texts may provide a "win-win-win" solution. If enough talented teachers consider contributing to them as a win rather than a financial loss, and are supported by universities in doing so, this may well be the case, and a selection of excellent print texts, Web texts, and wiki texts will be available. At the very least, ethical issues that arise when adopting

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a self-written text, ones which most professors would like to avoid, will not be germane with wiki texts.

There is widespread controversy about electronic textbooks that have been recently introduced (*20*). Examples are Macmillan's "DynamicBooks", and others which have similar features. The books can be modified by instructors and annotated by students, but their use is usually limited to a set time period, and the book self-destructs after a semester or a year. The limited availability would seem to be a requirement, since there is no formal citation requirement for sources of additions or revisions, and there is no public scrutiny of the accuracy of additions. DynamicBooks rely solely on readers to detect errors in the text. Commentators have pointed out the risks (*21*). The ChemPRIME model avoids this problem by allowing all registered users to edit entries. Integrity can be maintained by using archived pages (see below) while a course is being offered. The wiki is freely accessible property to all users without time limit.

Many publishers have similar ebooks (*22*) but they have different software platforms, so users need to learn idiosyncratic commands and markup. By standardizing on the MediaWiki markup, standard for Wikipedia®, ChemPRIME avoids that frustration.

The ChemPRIME wiki text is free (like Wikibooks®) and subscribes to the "Creative Commons" licensing convention (*23*). This publishing model depends on faculty who are willing to develop course materials that are accurate and well-written. Some universities support faculty who consider this work as part of their job, but many faculty have insufficient time to produce course materials. Part of the reason publishers find ancillaries profitable is that close to 50% of U.S. faculty are temporary, so they may not be willing, or able, to contribute to free courseware development as part of their job as teachers. The success of Wikipedia, however, suggests that contributors can sustain such an effort, even the number of contributors is small compared to the number of users. ChemPRIME, like most wikis, records all contributions, so that proper attribution is guaranteed. An immutable record promotes acknowledgment of this as professional activity and may help assure appropriate academic reward. The "History" tab associated with each page contains a record of all contributors. A wiki book has the potential to have many qualified editors, because all users are potential editors. In the early stages, revisions to ChemPRIME will be tracked and vetted, but we assume that with expanded use, errors will be corrected as efficiently by all users as they are in Wikipedia. Wikipedia has an error rate similar to that of the Encyclopedia Britannica according to a 2006 article in Nature (*24*). A recent ACS Webinar discussed the advantages of "Crowdsourcing" (*25*), and we hope that a structured wiki text like ChemPRIME will be attractive to users and contributors.

One of Koch's recommendations is to patronize the Creative Commons (*26*), but he concludes that, in spite of its advantages to students and the educational enterprise in general, this approach is unlikely to interest textbook authors.

ChemPRIME is part of the Chemical Education Digital Library (ChemEd DL) (*27*) and the National Science Digital Library (NSDL), so it is dependent on government support. It is possible that advertisements may support ChemPRIME (even some ebook publishers are considering them for additional income), but advertisements may be an undesirable distraction. It may be that government funding for teaching materials will increase; for example, a bill was proposed in California to use revenue from the state lottery to establish open education resource centers (*28*). Since several states have legislated mechanisms to abate increases in textbook prices, it may be inevitable that there will be government controls of some kind. Continued participation through NSDL seems particularly reasonable and appropriate, since the educational system in the U.S. is otherwise mostly a not-for-profit enterprise.

A wiki text evolves gradually, thus avoiding the frequent revisions of texts that publishers feel is necessary to maximize profits. Given the chain of oligopolistic publishers, distributors, and universities who are reluctant to forfeit their revenue stream from the sale of new books, it is unlikely that the situation with printed texts will change. Many faculty agree with James K. Stock of Harvard that "New editions are to a considerable extent simply another tool used by publishers and textbook authors to maintain their revenue stream, that is, to keep up prices" (*18*), although publishers claim that faculty want new editions. A wiki text grows incrementally, and in the case of ChemPRIME, by adding novel Exemplars, so it avoids the “New Edition” problem while maintaining currency. Other wikibooks are under development, but they are relatively unstructured compared to ChemPRIME ((*29*, *30*))

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Toward Improved Pedagogy

As suggested above, ChemPRIME allows for a logical development of principles and a case-study, “top down” approach at the same time, so it should answer the student complaint of “irrelevance”. As Willingham (*31*) points out in “*WhyDon’t Students like School*”, “...In other words, it’s the content that matters. We’re curious about some stuff but not about other stuff.”

But relevance is not enough to drive interest, as Willingham also points out. Interest is maintained when new information is connected to previous knowledge, and at a similar or slightly higher level. It’s critically important that students have the appropriate prerequisite knowledge, at the appropriate level. Exemplars will not be interesting or engaging if they aren’t presented in a manner that allows logical, coherent development of concepts. If exemplars are too challenging, students say to themselves “I’ll never understand this”, and they see nothing but frustration in trying. Nor will they be interesting if they’re not challenging enough, because students will not see any intellectual satisfaction in reading them. These are the reasons why Wikipedia® isn’t a good textbook, although it consists of readily accessible, mostly accurate information, and why “Googling” topics, or viewing other Web texts may be frustrating to students.

ChemPRIME presents Exemplars in an order dictated by logical development of concepts. Without this structure, it is very difficult to develop “case study” approaches, because the cases, while engaging to students, typically require prerequisite knowledge that must be supplied “just in time” rather than developed through logical relationships between concepts.

We don’t intend to limit the ability of students or faculty to change the sequence of topics. Many CoreChem chapters can be interchanged while still supplying the appropriate prerequisite knowledge for each topic. Exemplars go along with the topics, so if the chosen chapter order is appropriate, so will be the selection of Exemplars. We feel that it's critically important to develop the wiki site around sound didactics and pedagogy, rather than as a repository of information. Learning is optimized when exciting ideas are presented in a coherent, logically developed manner.

ChemPRIME's organization around concepts is, of course, supported by learning research. Several recent reports indicate that students' understanding of a subject can be constructed more effectively if the conceptual structure common to experienced practitioners forms the basis for organization of content. For example, the first of seven principles of learning promulgated by the National Academies of Science (NAS) (*32*) states, "*Learning with understanding is facilitated when new and existing knowledge is structured around the major concepts and principles of the discipline.*" When students know that a quiz on the enthalpy of fusion may have questions on anything from the "Amazing Ice Diet" to the cooling of plutons (vide supra), they are forced to see that "Abstraction is the goal of schooling" (*33*). We want students to be able to solve new problems, and avoid the kind of memorization where students can calculate the amount of heat needed to melt an ice cube, but can't imagine how to calculate the heat released when a kilogram of magma solidifies. In *How Students Learn*, Donovan and Bransford point out that "Using concepts to organize information stored in memory allows for much more effective retrieval and application" (*34*).

As a result of the organization of Exemplars in a conceptually coherent way, ChemPRIME fosters metacognitive strategies (*35*) which appear to be critical to learning chemistry (*36*). It develops the ability of students to recognize and learn underlying concepts, and discourags the tendency to memorize particulars. When students see a menu of exemplars like the ones above for enthalpy of phase changes, they should realize that there is an underlying abstract or generic idea (a concept) that they should extract from the particular instances. Quizzes will presumably be either content neutral, or constructed from a randomly chosen Exemplar, so students will begin to extract general concepts in order to succeed. This is different from simply reading a selection, because it involves evaluation of what is gained from the readings and self-monitoring, which are metacognitive processes.

ChemPRIME is consistent with constructivist ideas. In ChemPRIME, concepts are developed sequentially or cumulatively (hierarchically). Each step builds on a foundation or scaffold of simpler ones, or as Willingham puts it, "Understanding is remembering in disguise" (*37*); every new idea must build on previous ideas. Exemplars are hung on this structure, avoiding the difficulties of "just in time" learning of principles. But it's very important that Exemplars present concepts in terms of concrete information of interest to students. "We understand new things in the context of things we already know, and most of what we know is concrete" (*33*) so learning new concepts in the terms of a familiar discipline may be helpful.

Exemplars provide an opportunity to incorporate recent chemical research and real-world applications in a course. Students are impatient to start dealing with real problems at the forefront of a field. For example, the Exemplar on phase

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change materials mentioned above introduces recent approaches to incorporating PCMs into architecture. PKAL summarizes our commitment to "*connect student learning in STEM fields to the world beyond the campus, so, with the help of capable teachers, students appreciate the relevance of their studies and consider careers that use the skills and understandings gained from study in these fields*" (*38*). Bridging the gap between theory/research and application was one of the themes of the initial Innovate America Report, and subsequent reports have reiterated the need for moving away from lecture-mode approaches in undergraduate STEM education. They emphasize the importance of increasing innovation and diversity in STEM education programs and the increasingly urgent need for change (*39*).

There is good evidence that embedding concepts in broader multidisciplinary contexts can foster learning (*40*), and it may be particularly important for nontraditional students. But learning through multiple exemplars may be used in the context of remediation as well: Students who do poorly on quizzes may succeed after viewing a concept through the lens of more than one exemplar. We've all experienced the difficulty of finding errors in our own writings or problem solutions when they're too familiar, and how much a fresh look at the work may help.

ChemPRIME is compatible with virtually any teaching method, but wikis in general seem particularly appropriate for Peer Led Team Learning approaches, and for individualized instruction in general.

All the "bells and whistles" of a modern chemistry course can be built into a wiki. We generally link to original sources for videos and much other media, but animations are easily included, and we will probably incorporate MediaWiki's® video capabilities. ChemPRIME has Jmol models, and of course the range of graphics suggested by the figures above.

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Practicalities: Using ChemPRIME in General Chemistry Courses

The ChemPRIME main page can be accessed by a Google® search on "ChemPRIME", or directly through its URL (*41*). Any of the pages mentioned in this chapter can be accessed by entering the page name or a keyword in the search box. Clicking on "Go" links to pages with that page name, while "Search" returns the names of all pages with instances of the terms entered.

The Use of Wikis

Wikis present a dilemma: The advantages of being open source and editable seem to be in conflict with the disadvantages of being susceptible to malicious editing, or simply erroneous but well-intentioned editing, while a course is in progress. How can students be held responsible for information that is in flux during a course? The resolution of this dilemma is outlined below.

The advantages of wikis in education have been noted (*42*). They are supported by the NSDL (*43*), and are enjoying increasing use in chemistry as reported in the 28th ConfChem proceedings (*42*, *44*). Results of using a wiki in chemistry courses have been reported (*45*, *46*). We have chosen MediaWiki because its editorial policies and techniques are so well established as the base for Wikipedia. MediaWiki is easily adopted and open-source, and it is the engine for the NSDL wiki with which we plan to be interoperable, as part of the ChemEd DL.

The ChemPRIME wiki can accommodate Jmol molecular models as described in our Help pages, and it's easy to incorporate a variety of media. Many resources on the Web subscribe to Creative Commons licensing, which means that they can be incorporated in the wiki as long as the source is cited.

The most important feature of wikis is their promotion of collaboration and cooperation. With careful guidance, students can write Exemplars, working individually or as teams on topics which engage them. Wikis seem to be the perfect platform for strategies that promote student active participation, either as teams or individuals. Students may create exemplars through a "Student Assignments" portal (see below) where they won't be immediately linked with other wiki pages, or, with faculty guidance, students may create exemplars in the usual way (see below).

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Sabotage-Proof Pages

One of the main concerns about teaching with a wiki is that documents will be corrupted, either intentionally or unintentionally, by users. This potential problem is easy to avoid, although it has not been a significant issue in our experience. At Kutztown University, we create the course schedule as a wiki page (*47*) with links to unalterable pages in ChemPRIME. At the University of Wisconsin, a separate content manager, Joomla® is used in much the same way (*48*) as described elsewhere in this volume. The solution is flexible: links to unalterable pages can be created in any HTML document.

Unalterable pages are stored in MediaWiki sites by "Revision Number". By navigating to any page, and clicking on the "History" tab, specific revisions (including the current version) of a page are displayed. If one is selected, the wiki displays the page and its URL, so the URL can be copied and pasted as a link or "anchor" in any HTML document. The URL contains a unique Revision Number for the page. If the page is altered, it will be assigned a new Revision Number, so the link will return the previous page, not the altered one. The Revision Number can be extracted automatically in an HTML document as explained in the ChemPRIME "Help For Contributors" page. We have not experienced any malicious alteration of pages by our students, but use a standard spam filter to prevent "bot" attacks in general. Students are allowed to create or modify pages after they register, so the username of anyone who alters a page is recorded, and, of course, the alteration is easily undone by standard wiki methods.

Order of Topics

Because there is some flexibility in the order of topics in the general chemistry course, the hyperlinked course outlines mentioned above offer a convenient way to organize topics. Hyperlinks to other readings on the Web can also be included where they are appropriate, but we have kept our schedule simple, preferring to include hyperlinks to additional information in the Tracks, or in PowerPoint slides that are presented during lectures. The slides are available in a local course management system.

Support for Contributors and Modifying Pages

ChemPRIME includes a "Help for Contributors" wiki page that has step-by-step instructions for creating Exemplars and incorporating graphics and Jmol molecular structures, and other editing resources. Most of the editing practices and policies in ChemPRIME are identical to those in Wikipedia, so Wikipedia Help pages can be used in addition to our own. Wikipedia help pages are accessed by entering Help: topic (for example "Help: Advanced Editing") in the Wikipedia search box. Wiki coding is not always simple, but the usefulness of wikis, not to mention the omnipresence of Wikipedia, suggest that learning how to edit wikis is a valuable, transferrable skill.

To create an Exemplar, we recommend copying the CoreChem page, creating a new page with the Exemplar name, and then pasting the copied text into the new page. The page can then be modified to include the new information, while any esoteric wiki code that is present can be used as a guide. This procedure helps guarantee that the same concepts will be presented in all Exemplars.

Online Quizzes

Questions have been selected for selected text sections of the ChemPRIME wiki, and are available for adoption by authenticated faculty on the ChemEd DL site (*49*) They are included in a Moodle® course which allows question files to be exported in formats used by other course management systems. The questions are meant to be secure, so they are appropriate for tests or student access by password only.

Activities at UA

Students in a non-majors "Chemistry and Society" course taught by Robert Belford at the University of Arkansas at Little Rock, have developed exemplars in ChemPRIME. Working as groups, students suggest (or are given) a story line, like nuclear waste for example, and asked to find the chapters in ChemPRIME which might provide relevant background information. They then create a copy of the ChemPRIME page, and edit it to develop their story line. Students are encouraged to include multimedia from online sources, to connect with non-chemist readers, but they must correctly evaluate the content in terms of the ChemPRIME chapter. Students compose five questions and answers about their story, which are edited by the instructor, and added to a final exam when appropriate. We created a simple entryway ("Student Assignments") (*50*) into ChemPRIME, where wiki page linking is limited during the editing process, for these student projects. It

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is also possible to employ “User:” pages or subpages for development of content, which is a standard MediaWiki practice.

The ChemPRIME Project

ChemPRIME rests on the foundation of the ChemEd DL administered by Jon Holmes at the University of Wisconsin/Madison. Justin M. Shorb, a graduate student in Chemical Education with John W. Moore at Madison, is the ChemPRIME wiki Systems Administrator, and in that role created much of the structure of the ChemPRIME wiki site, including templates, wiki extensions, the Jmol interface, and spam filters. Justin coordinated much of the work at UW. Xavier Prat-Resina, a UW postdoctoral fellow in Chemical Education with John Moore, worked with Justin to build the Jmol interface with the Molecules 360 database of the ChemEd DL. The CoreChem pages were adopted from the Moore, Davies, and Collins text principally by Juliane Ober (JCE and ChemEd DL Staff), with help by a cadre of undergraduates, including Adam Hahn and Tim Wendorff working mostly on wiki editing, and Greg Sovinski working on image attributions and metadata. Robert E. Belford at UALR has guided students in creating exemplars, and Sofia Erazo (UW graduate student in Food Science) has worked on exemplars in the Food Track. Jeff Curless (senior undergraduate at UW) has been the point person for Moodle question bank development.

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Conclusions

ChemPRIME reflects the changes in the chemistry discipline by developing a new didactics of chemistry, which by happy coincidence fulfills the recommendations of many contemporary educators. ChemPRIME allows students to study topics that interest them, but maintains a logical development of concepts. It is a wiki text that marries a truly open source structure with the potential for accuracy typified by Wikipedia. In particular, this approach avoids some of the problems associated with printed texts, allowing incremental improvements rather than frequent new editions, while keeping the cost low. Wikis allow customization for a particular group, and promote student involvement in creation of textual materials.

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Chapter 15

The ChemPaths Student Portal: Making an Online Textbook More than a Book Online

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The ChemPaths Student Portal is more than just an online textbook, it incorporates linked problems, multimedia, and interactive 3-D structures. ChemPaths also incorporates navigation that takes advantage of research in hypertext learning. In addition to describing the development and use of ChemPaths in courses, this chapter describes the theoretical basis for its design. These stem from research in chemical education, hypertext learning, and applied constructivist theories. The chapter concludes with twenty questions intended to guide the reader in the design and use of digital textbook substitutes.

Background

Around 1440, Johannes Gutenberg revolutionized the distribution of knowledge by inventing the modern printing press (*1*). Books became more affordable and therefore more widespread. Learners for the first time could actually have their own copy of a book to study, read and carry with them to their courses. Today, in 2010, we are experimenting with ways to take physical textbooks out of students' hands and replace them with ever-changing and evolving online gadgets that access knowledge held both nowhere and everywhere (*2*, *3*).

The goal of today's education innovators is to forge a pattern of behavior in this new online milieu. The architecture of a book is so engrained in our culture that thinking outside of this particular rectangular prism can prove to be daunting (*4*). The publishing industry has evolved from Gutenberg with his press to a multi-billion dollar business. From manuscript to final distribution, a

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

published textbook passes under hundreds of eyes before the first student opens it on the first day of school. Those eyes check both form and content in hopes of maximizing the learning experience. There is an unconscious aligning with standard practices within the textbook world that keeps a traditional table of contents and chapter/section hierarchy. This structure is time-tested to the point where we rarely question its superiority over other architectures (*5*).

Today, dedicated individuals with access to a server, time for development, and knowledge of HTML can create their own set of learning resources according to their own desired architecture. This can be linear (like a traditional book), extensively interconnected, or module-based. It is important to realize the extent to which Web-based development enables cost-effective and rapid implementation of learning resources (*6*). It is also important to realize that learning materials are being made available to students with less review than ever before and often are being developed without taking advantage of all of the available research in chemical education, in educational psychology, in hypertext learning, and in accessibility standards.

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For instance, in a review reporting a meta-analysis of science education research, Wu and Shah state five design principles that should guide development (*7*):

1. Providing multiple representations and descriptions,
2. Making linked referential connections visible,
3. Presenting the dynamic and interactive nature of chemistry,
4. Promoting the transformation between 2-D and 3-D, and
5. Reducing cognitive load by making information explicit and integrating information for students.

The development of many learning objects available on the Web today has not been informed by such guidelines, and many developers may not even be aware of them.

ChemPaths represents our best effort to bring these facets together into a single project. It is meant to continue to evolve and be a *living* textbook—a place where students (and teachers) can go to find excellent learning materials for every topic of introductory chemistry (*8*). ChemPaths began as a digitized copy of *Chemistry* by John W. Moore, William G. Davies and Ronald W. Collins (*9*). A team of editors then moved the text to the ChemPRIME wiki (*3*, *10*), updating the language and content. For instance, multiple representations of concepts were provided using interactive molecule viewers, embedded movies, and animations. Examples were updated with more modern approaches. Intra-text references to other sections or pages were replaced with links, and whenever possible 2-D and 3-D structures were used. The editing team collaboratively reviewed each other's work to build concise and integrated content in the wiki.

Simultaneously, a Web site, ChemPaths (http://chemed.chem.wisc.edu/chempaths) was built to facilitate student navigation. Thus, while the text itself was and continues to be developed using the rapid versioning and editing platform of a wiki, the student interface was built using a tool much better suited to hypertext learning. This tool allows more than one approach to developing

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a learning module, enabling different instructors to design different ways for students to interact with content. The tool also enables navigation based on constructionist principles applied to the use of hypertext to enhance learning. Because the entirety of text, multimedia, and other learning materials is available online, a teacher can display example molecular structures or videos directly from the text during class, thereby more fully integrating the online textbook into the course.

Prior to the development of ChemPaths we used a course management system to make up homework assignments by choosing questions from a large pool of similar questions (the *JCE* QBank General Chemistry questions, (*11*)). Each student had a unique homework assignment. When a student submitted homework, the student was provided feedback that suggested which part of the printed textbook to study if the student had answered incorrectly or felt unsure about a topic. For ChemPaths the feedback was rewritten so that the student is directed via a hyperlink to the appropriate section of the online textbook. This further integrates the reading with the practice problems.

This whole interlinked system, which affords continuous intellectual travel through text, tutorials, chemical demonstrations, and homework, is what we call ChemPaths. Every aspect of this online portal has been developed with open source software to encourage collaborative development work. Our content is distributed under a Creative Commons License so that submissions are usable freely under multiple platforms (*12–16*).

The rest of this chapter illustrates what constitutes an electronically-deliverable integrated learning system (online textbook), what educational and design challenges must be addressed, and how ChemPaths has addressed these challenges. We report specifically our experience developing and using such a system for a general chemistry course. It is our hope that the reader will more fully understand what concerns should govern the development and choice of an online textbook for any course.

Examples of Textbooks Delivered Electronically

ChemPaths has been developed to be a multifaceted approach to online learning that can supersede the traditional textbook. For purposes of comparison, it is useful to provide some basic vocabulary and to highlight a few related approaches to electronic delivery of general chemistry textbooks.

- eBook—a standard hardcopy book that has been turned into a digital format. Examples include PDF scans of current hardcopy books, books online that only have one direction to read (next page, previous page), and many books available for e-readers (*2*, *17*).
- e^{2}Book—an eBook with a more dynamic architecture. According to Lubliner, there are four criteria for being an e^{2}Book. First, links within the text point internally or externally. Second, the format of the book can be transformed to meet the needs of students or instructors without changing the exact content. Third and fourth, multimedia and semantic

terminology are used, frequently linking to a digital library or content repository (*2*).

- Online Textbook—a Web site that has been designed to be a complete substitute for the traditional role of a hardcopy textbook. An online textbook replaces a hardcopy textbook; a course using an online textbook does not need a hardcopy book. An Online Textbook can be either an eBook or an e^2Book, depending on its use of hypertext.

In the next few sections, descriptions of various substitutes for hardcopy textbooks are listed in approximate succession from those built with more traditional architectures to those using more dynamic architectures (*4*). This is only a sampling of various types of sites or resources available; it is not an exhaustive list.

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eBooks

On many of today's eBook readers such as Kindle, or the iPad, exact copies of some traditional hardcopy texts are available (*2*, *17*). These typically have the same linear architecture as the original books, possibly with the addition of a search feature. Some of these readers support file formats with moving images (video clips or animations). In the future, these will likely have the ability to incorporate more interactive features.

Wikibooks

The Wikibooks Web site is a part of the family of wikis managed by the Wikimedia Foundation, of which Wikipedia is also a member (*18*, *19*). Given the architecture of a wiki, this site has frequent in-text links to encyclopedic-style information pages that comprise the Wikipedia site. The pages have been linked into a linear book-like structure that students can navigate much like an ebook. Authors can freely edit any page, which allows for rapid development of content. However, such freedom can be abused by vandalism or intentionally misleading edits. Therefore, Wikibooks has instituted the "Flagged Revisions" extension. This means that an editor must accept any change or revision before it becomes live for the general public. Also, the public (or students) view only the most recent accepted version. At the time of writing, however, very few pages have any accepted revisions and Wikibooks seems to have stagnated.

An Introduction to Chemistry by Mark Bishop

Bishop has developed an excellent online book that is also available in printed form (*20*). To address a critical difference between pedagogies, he has written two versions of the online book: one that introduces chemistry from an "Atoms First" approach and another that uses a "Chemistry First" approach. Each book has a

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table of contents, chapters with sections, and helpful chapter supplements. The multimedia objects have been embedded or included in helpful interactive flash tutorials. The text includes voice-overs to engage readers in active learning, as well. Bishop has created an excellent eBook that extends the traditional textbook into the world of multimedia in a notable way and exemplifies the features of an eBook.

DynamicBooks by Macmillan

DyanamicBooks is an effort by Macmillan Publishing to forge into the new digital era of publishing (*21*). Instructors are able to put together snippets from various books published by Macmillan, along with self-authored notes, corrections, or addenda. The students can then purchase these as eBooks. This is an effort to bring the benefits of crowd-sourcing and collaborative work into the publishing community while still maintaining editorial control over the material that is sold as 'published.'

Connexions

The Connexions Project was initiated at Rice University to build an interconnected curriculum across not only a single course, but among courses (*6*, *22*). It utilizes a connected module architecture where authors build a module that teaches a given topic. Instructors can then build chapters or courses out of these content modules. Schools, departments or instructors can build sets of modules or collections they have reviewed. These accepted versions could then become part of what Connexions calls that institution's or instructor's "lens." Browsing these lenses is a way to find reviewed learning materials. This site has been developed with the spirit of peer collaboration and generating a community of learning. Connexions has also built a set of authoring tools that enable rapid contributions. Currently Connexions has only one chemistry module (textbook) available, written in 2007 by John Hutchinson (*23*). The whole site is available freely to anyone.

ChemPaths: Learning to Meander

The Chemical Education Digital Library (ChemEd DL) houses collections of videos, animations, images, assessment questions, and molecular structures within its database (*24*). As part of the NSF National STEM Education Distributed Learning (NSDL) project, the ChemEd DL was challenged "to investigate the relationship between design of collections and their utilization by instructors and students" (*25*). ChemEd DL interprets this to mean building from its content collections larger assemblages that will be useful in instruction. NSDL is striving to not only curate collections of multimedia objects and data, but to provide these materials in a pedagogically useful manner. This interconnected and highly linked architecture, along with its connection to the ChemEd DL brings ChemPaths into the realm of an e^{2}Book.

ChemPaths is our approach to building a next-generation chemistry textbook within the online world (*8*). The following description of building this student portal begins with a look at how the architecture of electronic media influences student learning. This is followed by a discussion of the interplay of navigational architecture and pedagogy. Finally we detail the content of ChemPaths and how it has been used within a general chemistry course.

Hypertext Learning

What Is Hypertext?

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What we casually call “the Internet” was once local copies of linked text pages with perhaps an image or two. Pioneering instructors proposed that the non-linear connections between text and images can have an effect on student learning (*26*). This non-linear organization of information was dubbed “hypertext” and in fact, HTML stands for “HyperText Markup Language.” This technology was never intended to be linear: a highlighted word links to a different page, which has a link that can bring you back to a page you have already read—or even take you off to yet another related topic or image.

Hypertext structure is exemplified within Wikipedia. A wiki is designed to connect information in an easy-to-edit fashion (*27*). We read until we happen upon a blue-underlined word that catches our eye and we click there. A new page opens that expands upon that topic and before we realize how much time has passed, a few more clicks and a few more topics have been explored. This haphazard structure is commonplace on wikis, news sites, and many topical Web sites. These sites, coupled with a Web search, constitute casual learning experiences that many of today’s students (and probably their instructors) have every day.

However, many instructors have become accustomed to oral story-telling, often through lecturing, which can be highly effective when done well. This linear thought process is clean, directed, and arrives nicely where the instructor intends to take the student. This conceptual framework has been routinely extended to textbooks and tutorials (*28*). An eBook is still trapped in this organizational structure. An underlying assumption is that a student’s personal schema needs to be challenged by specific prior information before the student can assimilate other, more complicated knowledge (*4*, *29*, *30*). In fact, in many cases this is probably true (*31*).

In some cases—and for some students—this linear organization can be a hindrance. For instance, many chemistry instructors prefer to teach orbitals before molecular structure while others prefer to derive basic molecular structure from experimental data and then talk about theory. There are benefits to both methodologies, but either the instructor must write his or her own book or do what nearly all instructors do: assign reading out of order with respect to the textbook’s table of contents. Students must then view material out of order when they read and may have to do the best they can with paragraphs that depend on background information to which they have not been exposed.

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Before we look at how hypertext can address the pitfalls mentioned regarding the use of a traditional textbook, we must first understand perceptions of knowledge as experts versus our students' needs when learning.

The Difference between Organization and Pedagogy

Experts and novices recognize the connections among concepts, graphics, text, and symbols in vastly different ways. In a study by Kozma and Russell, it was shown that experts find larger groupings among related images, graphs and videos than do novices (*32*). This may seem intuitive and come as no great shock as similar work was done in 1983 by Johnstone (*33*), but it can be overlooked when designing an online chemistry textbook. While an author may intuitively make the links between various concepts within a textbook, students will likely not. Therefore the designer of an online textbook should strive to reinforce the conceptual connections inherent in an expert's understanding by putting the content together in a purposeful way with meaningful links. This can aid the student in seeing how an expert might view the material.

Yang has presented guidelines for incorporating constructivist theories into the design of a hypertext (or hypermedia) document (*34*). The framework of a hypermedia system architecture can be described within each of three constructivist perspectives: semiotic, cognitive, and social. The list of features is extensive, and is elucidated later in this chapter. However, it is important to recognize that the architecture of hypertext is well-aligned with constructivist learning theories.

In addition, Dillon *et al.* specifically discuss the nature of navigation within a hypertext using "Schema Theory"—which is closely coupled with Constructionist Theory (*4*). The idea is that navigation options impose structure onto a learner's schema. Thus, as a student learns chemistry it is important that the connections the student builds reflect correctly the conceptual connections an instructor is trying to convey. That is, navigation is another way to either reinforce or weaken constructed schemas. Hypertext was seen as early as 1985 with the SuperBook project as a mechanism to allow students to more actively engage while learning from textbook-like materials (*26*, *35*). Therefore it should be beneficial to incorporate similar navigational structure to reinforce student learning.

Example within ChemPaths

Early in the development of ChemPaths it was decided to deliver our content through the browser as a Web site, not as a downloadable pdf or as an eBook. As new devices come onto the market they almost invariably include a Web browser, thereby making ChemPaths available in many more places than would be possible if it were based on proprietary hardware such as an eBook reader.

ChemPaths partners with the ChemPRIME (Chemical Principles through Integrated Multiple Exemplars) project, which uses the MediaWiki engine to build the majority of the content (*3*, *10*). (Edward Vitz discusses the development of the ChemPRIME project in another chapter in this book.) In brief, authors can easily build pages that link together like Wikipedia, or the Wikibook mentioned earlier.

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For example, we entered the entire textbook, *Chemistry*, by Moore, Davies, and Collins, into the ChemPRIME wiki in a relatively short time. However, navigation through such wiki pages is currently either completely uncontrolled (like Wikipedia) or linearly controlled (like Wikibooks or other online texts). Neither extreme takes full advantage of the features of a learning tool built using hypertext. There is also the issue of uncontrolled editing of a wiki, which has the potential to make the textbook different each time a student reviews a topic.

Because of the problems with navigation in a wiki and the pedagogical importance of navigation, we decided to build a structured, yet relatively free, mode of navigation. ChemPaths, the site students interact with, was built using the Joomla! content management system as a front-end (*12*). This enabled custom functionality that allows students to have a semi-structured reading experience. The navigation is akin to a pathway through a lawn along stepping-stones. At each stone, students can deviate from the path in several directions, but the main thoroughfare is always identified. This enables students to return easily to the instructor-designed pathway through the material.

The ChemPaths layout in Figure 1 represents a typical page on conversion factors (*36*). The left side-bar is a table of contents; each chapter title can be clicked to show the section headings contained within the chapter. From the expanded table of contents, it can be seen that this page, “Conversion Factors”, is the next to last section of the first chapter, “Introduction”. The right side-bar contains related textbook pages and other tutorial pages as well as links to pages that represent applications of conversion factors in biology, everyday life, forensics, and several other fields. These are exemplars from the ChemPRIME project.

At the top of the page are tabs that link to the ChemPaths home page, to an interactive periodic table (Periodic Table Live!), to the full table of contents of the *Chemistry* textbook, and to Quick Resources (a glossary and tables of data). Within the text, some words are highlighted; these can take a student to related textbook pages or they can open tutorial pages on conversion factors; other highlights can expand images for more detail.

The next stepping-stone along the path is always available as an option from any page and is always at the lower right corner of the page. In Figure 1, this next step is the page called “Impact,” which is the last page in the “Introduction” chapter (see the table of contents in the left side-bar). The interface is designed so that when a link to a related page is clicked, the page opens in the same window with the same navigation aids in the left side-bar, in the tabs, and at the bottom of the page. Thus a student can explore new content within a familiar context. A student can elect to view a related page or explore multiple links to other pages, all while maintaining a guided navigation that is available whenever the student is ready to continue along the main path.

We refer to this navigation as “Learning to Meander,” but it might well be reversed to read “Meandering to Learn.” Later in this chapter we discuss specifically how students interact with this site on a daily basis. As you read this chapter, we encourage you to visit the pages mentioned. The URLs are included in the references and within the text as they are discussed.

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Interactivity

Theoretical Framework

Within constructivist theory, interactive learning objects receive due praise (*29, 30*). Interactivity encourages students to engage with the material and to actively construct their understanding of the material. This is not just theoretical; there is a good deal of research that supports the benefits of interactive practices in teaching chemistry. For example, Williamson and Abraham present an argument for interaction with animations in lecture and in individual settings. They find that learning gains are greater when animations are used (*37*). Barnea and Dori explore the use of multiple types of computer models and find that students who use such models have greater learning gains (*38*). For a good overview of incorporating visualization and interactivity into chemical education practice and design, we refer the reader to the review by Wu and Shah (*7*).

Example within ChemPaths

ChemPaths currently has more than 50 embedded videos and animations. Embedding the videos or animations within text with instructions to pause or play at given moments makes the words come alive and helps illustrate the dynamic nature of chemistry. Additionally, to actively engage the learner and help to connect 2-D representations with 3-D molecular structures, fully interactive Jmol structures of molecules are used whenever possible alongside traditional representations. The ChemEd DL Models 360 collection contains nearly 1000 Jmol structures at the date of this writing; new ones are being added continually (*13*). As molecules are added, *ab initio* calculations are performed to generate molecular orbitals, charge distributions, dipoles, vibrational modes and more. Each of these properties can be included in or excluded from the interactive viewer as part of a menu. The text walks students through the menu options and has them view the HOMO and LUMO when learning about MO theory, for instance. There is also ample opportunity to include external tutorials and interactive flash sites into an instructor's pathway, although so far only a few of these have been incorporated in the textbook pages themselves. As the ChemEd DL expands its arsenal of teaching tools to include more interactive learning objects, ChemPaths will expand to take advantage of them.

Contextualization

Context-Based Approaches

Teaching chemical concepts within a context-based approach is not new (*39*). Most textbooks have inserts that give real-world examples, or even a running theme such as *Chemistry for the Life Sciences*, where all of the examples are taken from a biological context (*40*). Bennett and Holman recommend that curriculum design involve choosing topics to reflect the interests of students within a specific course (*39*). Thus, a general-chemistry book that teaches within the context of biology is beneficial in a course where nearly all students have

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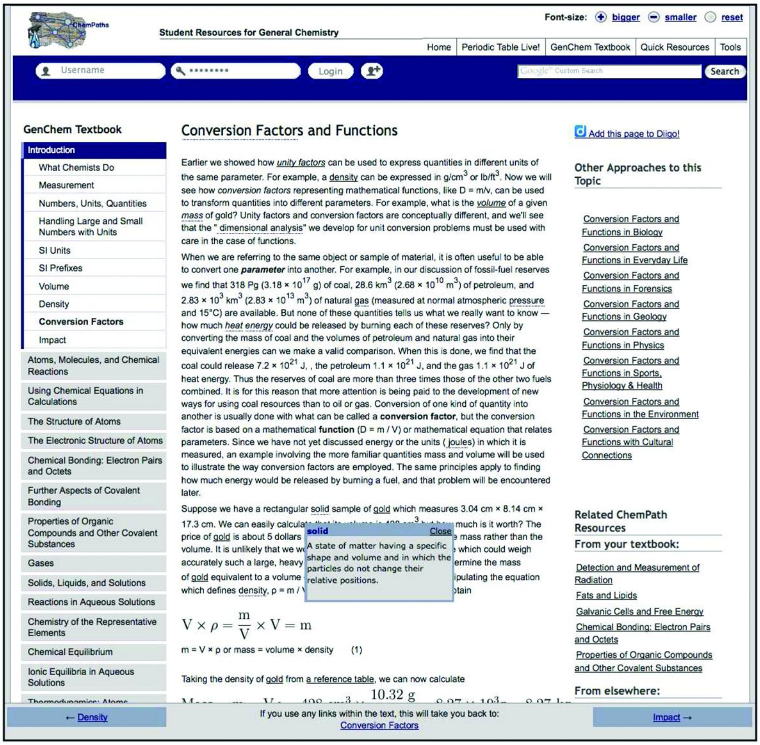
ChemPaths
Student Resources for General Chemistry
Font-size: bigger smaller reset
Home
Periodic Table Live!
GenChem Textbook
Quick Resources
Tools
Username
Login
Search
GenChem Textbook
Introduction
What Chemists Do
Measurement
Numbers, Units, Quantities
Handling Large and Small Numbers with Units
SI Units
SI Prefixes
Volume
Density
Conversion Factors
Impact
Atoms, Molecules, and Chemical Reactions
Using Chemical Equations in Calculations
The Structure of Atoms
The Electronic Structure of Atoms
Chemical Bonding: Electron Pairs and Octets
Further Aspects of Covalent Bonding
Properties of Organic Compounds and Other Covalent Substances
Gases
Solids, Liquids, and Solutions
Reactions in Aqueous Solutions
Chemistry of the Representative Elements
Chemical Equilibrium
Ionic Equilibria in Aqueous Solutions
Add this page to Diigo!
Other Approaches to this Topic
Conversion Factors and Functions in Biology
Conversion Factors and Functions in Everyday Life
Conversion Factors and Functions in Forensics
Conversion Factors and Functions in Geology
Conversion Factors and Functions in Physics
Conversion Factors and Functions in Sports, Physiology & Health
Conversion Factors and Functions in the Environment
Conversion Factors and Functions with Cultural Connections
Related ChemPath Resources
From your textbook:
Detection and Measurement of Radiation
Fats and Lipids
Galvanic Cells and Free Energy
Chemical Bonding: Electron Pairs and Octets
Properties of Organic Compounds and Other Covalent Substances
From elsewhere:
← Density
Impact →

Conversion Factors and Functions

Earlier we showed how *unity factors* can be used to express quantities in different units of the same parameter. For example, a density can be expressed in g/cm^3 or lb/ft^3. Now we will see how *conversion factors* representing mathematical functions, like D = m/v, can be used to transform quantities into different parameters. For example, what is the *volume* of a given *mass* of gold? Unity factors and conversion factors are conceptually different, and we'll see that the " dimensional analysis" we develop for unit conversion problems must be used with care in the case of functions.

When we are referring to the same object or sample of material, it is often useful to be able to convert one ***parameter*** into another. For example, in our discussion of fossil-fuel reserves we find that 318 Pg (3.18×10^{17} g) of coal, 28.6 km^3 (2.68×10^{10} m^3) of petroleum, and 2.83×10^3 km^3 (2.83×10^{13} m^3) of natural gas (measured at normal atmospheric pressure and 15°C) are available. But none of these quantities tells us what we really want to know — how much *heat energy* could be released by burning each of these reserves? Only by converting the mass of coal and the volumes of petroleum and natural gas into their equivalent energies can we make a valid comparison. When this is done, we find that the coal could release 7.2×10^{21} J, , the petroleum 1.1×10^{21} J, and the gas 1.1×10^{21} J of heat energy. Thus the reserves of coal are more than three times those of the other two fuels combined. It is for this reason that more attention is being paid to the development of new ways for using coal resources than to oil or gas. Conversion of one kind of quantity into another is usually done with what can be called a **conversion factor**, but the conversion factor is based on a mathematical **function** (D = m / V) or mathematical equation that relates parameters. Since we have not yet discussed energy or the units (joules) in which it is measured, an example involving the more familiar quantities mass and volume will be used to illustrate the way conversion factors are employed. The same principles apply to finding how much energy would be released by burning a fuel, and that problem will be encountered later.

Suppose we have a rectangular solid sample of gold which measures 3.04 cm × 8.14 cm × 17.3 cm. We can easily calcula much is it worth? The price of gold is about 5 dollars e mass rather than the volume. It is unlikely that we w which could weigh accurately such a large, heavy ermine the mass of gold equivalent to a volume ipulating the equation which defines density, ρ = m / V tain

solid Close
A state of matter having a specific shape and volume and in which the particles do not change their relative positions.

$$V \times \rho = \frac{m}{V} \times V = m$$

m = V × ρ or mass = volume × density (1)

Taking the density of gold from a reference table, we can now calculate

If you use any links within the text, this will take you back to:
Conversion Factors

Figure 1. Screenshot of a typical textbook page (36). A typical expandable table of contents is in the left side-bar. In the right side-bar are opportunities for exploration: "Other Approaches to this Topic" (which link to other tracks from ChemPRIME) (3), and "Related ChemPath Resources" from the textbook itself as well as other sources, such as tutorials. The bottom of the screen is devoted to navigation to the previous page ("Density", on the left), back to this page (center), and to the next page ("Impact", right). Tabs at the top of the screen allow access to resources such as a periodic table, a glossary, and tables of data. Hovering the mouse over a word included in the glossary (59) brings up a definition box (shown for the word "solid"). Intra-text links go to other parts of the textbook, such as the page on "unity factors" in the first line. When links are followed, the navigation at the bottom of the screen does not change, allowing students a quick return to the pathway.

an interest in biological science but is inappropriate for use in a course where half the students are engineering majors. A truly customizable textbook should then have a ready-made stockpile of identical concepts taught from within various contexts. Thus one semester an instructor can include the topic of acid dissociation constants within the context of biology. The next semester geology, or environmental science might be the context. To accommodate interests of subgroups of students in a large course, students with an interest in biological sciences could study topics in a biology track while students with an interest in environmental science could study the same topics but in an environmental track. Thus a course could be tailored to current events, scientific advances, and different interests of different student cohorts.

Example within ChemPaths

Contextualization of the chemistry concepts is done within our partner project, ChemPRIME (*3*, *10*), which is working to rewrite each section of a general chemistry textbook within the context of various "tracks." At present ChemPRIME includes these tracks: Chemistry in Geology, in Physics and Astronomy, in Everyday Life, in Foods, in Sports, Physiology & Health, in Biology, and Culture, in Environmental/Green Chemistry, in Forensics and in Lecture Demonstrations. In the ChemPRIME wiki, an exemplar of the topic can be added in each of these categories. The exemplars are stored in the ChemPRIME wiki and from there can be selected by an instructor using ChemPaths. This provides students with the option of learning the same chemistry concepts but embedded in a broad range of contexts. A team of dedicated individuals is currently adding exemplars at a rapid rate. As each new exemplar is added, it becomes available to students as a "Related ChemPath Resource" that can be viewed from any textbook page or can be included as part of the instructor's pathway through the material.

For instance, after discussing Gibbs energy, some traditional textbooks have a separate section on Gibbs energy with relation to coupling of biochemical reactions. The ChemPaths textbook does not necessarily include such a section; instead, Gibbs energy and coupled reactions is an exemplar in the ChemPRIME biological track. An instructor could construct a path to include this exemplar explicitly or the instructor could provide the exemplar as a link to a related ChemPaths resource in the right side-bar. If—or when—the general chemistry curriculum begins to emphasize molecular machines more strongly, instructors may choose to use a nanotechnology exemplar for that topic. Note, however, that the standard general-chemistry treatment and all of the exemplars are always available to be explored by any student meandering within the ChemPaths structure.

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The Triplet Relationship

Theoretical Framework

In addition to applying theoretical foundations to building the navigation of an online textbook, it is important to recognize the importance of the layout of individual pages. Since Johnstone introduced the triplet relationship (*41*) between the three levels of chemistry (macro, submicroscopic and symbolic), there has been a focus in chemical education to assess student understanding at each of the three levels (*42*, *43*). It is becoming increasingly clear that students need to conceive of the phenomenon being studied at all three levels in order to fully grasp chemical concepts.

As an illustration, Harrison and Treagust discuss student understanding of the particulate nature of matter (*44*). One study cited therein finds that middle school students commonly believe that matter is lost upon changing phase from solid to liquid (*45*). This misconception is also held by undergraduate pre-service teachers despite further learning in the sciences (*46*). This confirms a consistent lack of understanding at the submicroscopic level.

Multimedia has a valuable role to play in presenting learners with various modes of representation (*47*, *48*). The review by Wu and Shah discussed earlier in this chapter indicates that providing multiple representations and making linked connections visible is important (*7*). Thus juxtaposing macro images, atomic-scale representations, and symbolic equations should be valuable in addressing misconceptions.

Proximity of objects on a page or screen can aid students in developing conceptual links, but including all three modes of representation for each concept is expensive in hardcopy. Also, the nature of a phenomenon is often such that it cannot readily be shown on the printed page but lends itself much better to using video or animation (to demonstrate motion, for example) (*49*, *50*). Hardcopy textbooks frequently come with CDs or online material that could very well help students (such as those who think that matter is lost during a phase change). The problem is that almost no students, in the course of their daily study of chemistry, actually use the online or CD portions of their text (*51*). Therefore it is useful to specifically include multimedia and link the media to text as a means for enhancing students' understanding of concepts so the multimedia become an integrated part of the learning experience.

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Example within ChemPaths

Consider learning about osmotic pressure. It is important that a student recognizes what is meant by osmotic pressure on a macroscopic, submicroscopic, and symbolic level. Therefore, in ChemPaths, students are given the equation relating osmotic pressure to macroscopic quantities, an image of how this pressure is observed in the real world, and an animation to depict how the pressure is caused by transmission of solvent molecules through a membrane (*52*). The relationships among these three levels of representation are described in the text that accompanies the equation and graphics.

Figure 2 shows a snapshot of the animation. It begins with the membrane aligned with the vertical dashed line. The motion of the molecules begins to push the membrane molecules away from center, tracked by the crosshairs. The solvent molecules are color coded to differentiate molecules initially on one side of the membrane from molecules initially on the other side. Solvent molecules (but not solute molecules) are seen to travel from one side of the membrane to the other. The number of molecules traveling from left to right is fewer than from right to left.

The unequal motion of solvent molecules is related to the height of the solvent in the image of the experimental setup. Lastly, the motion of molecules and concentration differences made visible by the animation and the image correlate with the variables in the symbolic equation $\Pi V = nRT$ that relates osmotic pressure to temperature and concentration. As the sections within the

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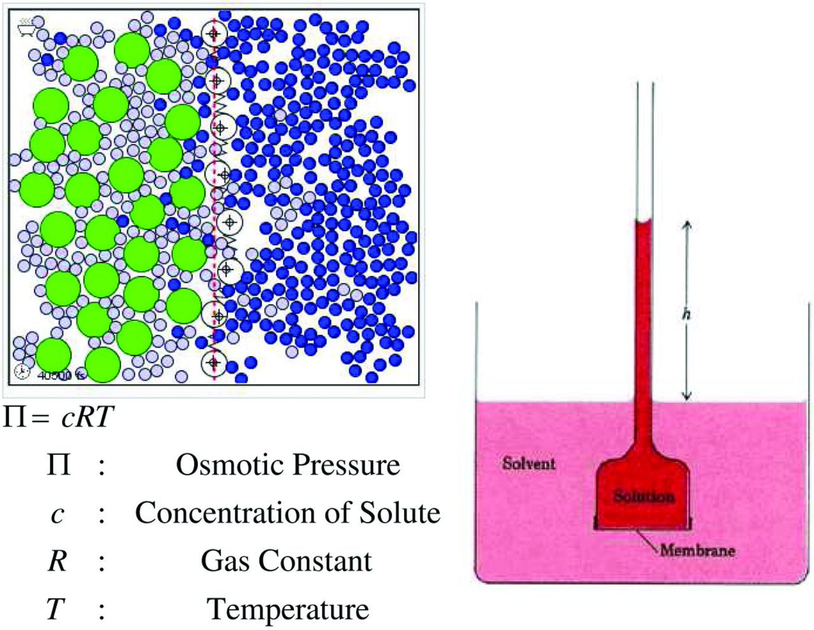

$\Pi = cRT$

Π : Osmotic Pressure

c : Concentration of Solute

R : Gas Constant

T : Temperature

Figure 2. This figure represents the Triplet Relationship as it is used within the page on Osmotic Pressure (8, 52). The student sees an image of the different levels of solution due to osmotic pressure, an animation of how osmotic pressure forces a membrane to deviate from its initial position, and also equation that ties the macroscopic parameters to the osmotic pressure.

text continue to be edited, this theoretical framework regarding multimedia and the triplet relationship guides the pedagogical development.

A Student Portal for Learning

The previous sections have described the theoretical frameworks and pedagogical concerns that need to be present in any discussion of building an online textbook. Included were examples of how these ideas have structured the development of ChemPaths. The rest of the chapter details the day-to-day operation of the textbook from the perspective of both students and instructor. Each group of students that used this site as their primary textbook elected a student board of representatives from each discussion section. These students met with the instructor each week to offer feedback and assist in the molding of the interface. Some design features reported in what follows were the result of student feedback.

Daily Pages and Pathways

Each day, students go to the ChemPaths Web site and click on their course, bringing up a navigation pathway specific for their course. The pathway is set up in advance by the instructor, who has considerable flexibility in its design. For the courses that have used ChemPaths so far, the pathway was based on work to be done for each day when there was a lecture in the course.

Figure 3 shows a screenshot after a student has selected the day of interest. Depending on assignments for a given day, the student is presented with links to course-specific sites for homework, quizzes, external tutorials, and lecture topics. (Because students in this course already had a printed textbook from an earlier course, alternate reading is given from the hardcopy textbook.) The instructor was free to invent his own pathway through the textbook, and a daily readings organization was selected to match the course organization.

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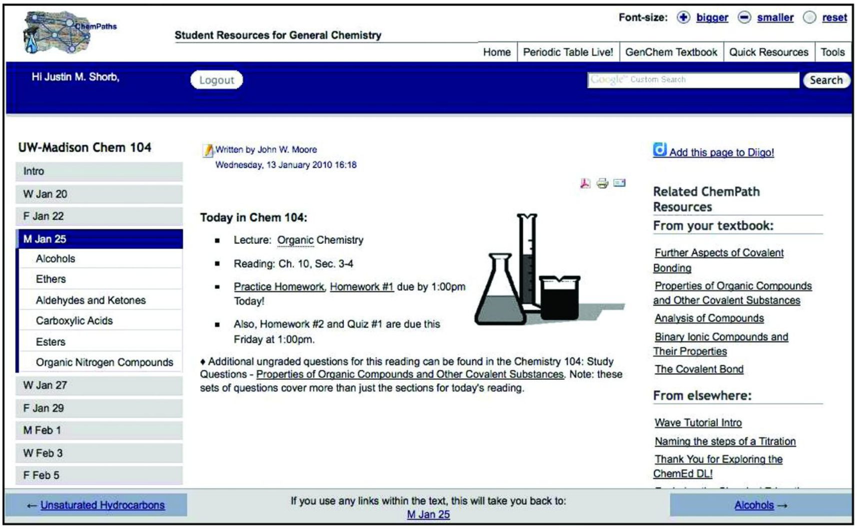
Meandering Navigation

At the bottom of the screen in Figure 3 is the main navigation bar, which allows the student to move along the stepping-stone pathway. At the left is a button labeled "Unsaturated Hydrocarbons" that goes to the previous page of reading (which was part of the material for Friday, January 22). At the right is a link to the next page of reading, "Alcohols". In the center is the statement, "If you use any links within the text, this will take you back to: M Jan 25". "M Jan 25" is the name of the current page and is a link to the current page. The student can click on any of the "Related ChemPath Resources" or any link within the text to visit other topics and still return easily to this page. The "UW-Madison Chem 104" pathway menu on the left, the navigation along the bottom, and the tabs at the upper right do not change when a related resource appears. Thus, students can feel free to click to enlarge an image, or click on the Periodic Table Live! tab to visit the periodic table page for an element such as sulfur, without losing their place along the pathway. A click on the link in the bottom center brings them back to the page that they were on before they departed from the stepping-stone path.

Student vs. Teacher

There is no requirement that a user log in to the ChemPaths Web site; the online textbook is freely available to everyone. If one does log in, the site becomes an instructor site. No screenshot is shown here because the differences in appearance are negligible. There are additional entries under "Related Items" that point to resources from the NSDL repository, and more editing information is given. Access is also granted to instructors to visit a forum, which is not yet active because there is currently little advanced usability granted to instructors. One of the main goals of the coming year is to develop the instructor interface to make building pathways from resources more user-friendly.

Textbook pages are being continually developed in ChemPRIME on the easy-to-edit Mediawiki platform. Therefore it is likely that pages used in a course will change while a course is underway because those pages have been edited by other users of ChemPRIME. To avoid students' having the disconcerting experience of seeing different information in the same textbook each time they view a specific page, ChemPaths acts as a "Flagged Revision" extension to the Mediawiki engine. That is, an instructor can control which version of a page in the ChemPRIME wiki


ChemPaths
Font-size: bigger smaller reset
Student Resources for General Chemistry
Home
Periodic Table Live!
GenChem Textbook
Quick Resources
Tools
Hi Justin M. Shorb,
Logout
Google Custom Search
Search
UW-Madison Chem 104
Intro
W Jan 20
F Jan 22
M Jan 25
Alcohols
Ethers
Aldehydes and Ketones
Carboxylic Acids
Esters
Organic Nitrogen Compounds
W Jan 27
F Jan 29
M Feb 1
W Feb 3
F Feb 5
Add this page to Diigo!
Related ChemPath Resources
From your textbook:
Further Aspects of Covalent Bonding
Properties of Organic Compounds and Other Covalent Substances
Analysis of Compounds
Binary Ionic Compounds and Their Properties
The Covalent Bond
From elsewhere:
Wave Tutorial Intro
Naming the steps of a Titration
Thank You for Exploring the ChemEd DL!
← Unsaturated Hydrocarbons
Alcohols →

Written by John W. Moore
Wednesday, 13 January 2010 16:18

Today in Chem 104:

- Lecture: Organic Chemistry
- Reading: Ch. 10, Sec. 3-4
- Practice Homework, Homework #1 due by 1:00pm Today!
- Also, Homework #2 and Quiz #1 are due this Friday at 1:00pm.

♦ Additional ungraded questions for this reading can be found in the Chemistry 104: Study Questions - Properties of Organic Compounds and Other Covalent Substances. Note: these sets of questions cover more than just the sections for today's reading.

If you use any links within the text, this will take you back to:
M Jan 25

Figure 3. Screenshot of a Daily Page within ChemPaths. The course readings are organized by day along the pathway at left, with navigation along the bottom.

will be included in the course. If more than one course is active, each instructor can decide whether to include a specific wiki page in his or her pathway, along with the exact date of the version of that page to include. Any edits that occur after that date will not modify that instructor's pathway pages unless the instructor changes the date of the version being used. This feature works both ways: new edits by others can be prevented from changing the ChemPaths textbook, but an instructor can make corrections and include them when necessary.

Lecture

Because instructors are in full control over the content of their textbooks, any digital material that they wish to use in a classroom can be incorporated into the textbook. For example, if an instructor wants to illustrate a topic in class with a video, the instructor can include the video on a page in the textbook. In the classroom the instructor can navigate to the ChemPaths site to view that textbook page and show the video. When students peruse the textbook individually, the same video shown in class is there, embedded in the text.

Diigo: Social Bookmarking

Each page of ChemPaths includes a link in the upper right corner, "Add this page to Diigo!" This link will bookmark the current page in a social bookmarking site, Diigo (http://www.diigo.com) (*53*). Social bookmarking sites allow students to keep a set of bookmarked pages and share their sets of bookmarks and comments with other members of a community. Diigo stands out in the social bookmarking arena because it is geared toward academics. It allows

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for bookmarking, tagging, highlighting, and adding sticky-notes. Each class that used ChemPaths was encouraged to use Diigo as well, and a class group was set up for students to share their comments with each other.

Anecdotes shared during the student board meetings indicate that students did make use of Diigo, although few shared their notes or highlights with others in the class group. Students reported that they used bookmarks to find where they had stopped reading so that they could continue on the same page the next time they studied. They used sticky notes instead of a separate notebook to annotate pages in the online textbook and marked sections to which they needed to return for further study. Others highlighted important sections of the text and one student found Diigo to be the most useful aspect of the online textbook.

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Assessment

Typically a general chemistry textbook contains a large number of sample problems at the end of each chapter. The digitized textbook also contained end-of-chapter questions, but these were used in a way that integrated them better into students' studying. Each course that has used ChemPaths has included a modified version of the *Journal of Chemical Education* Digital Library QBank collection of quiz and homework questions suitable for delivery by course management systems (*11*). QBank consists of a large number of sets of questions. Each set consists of from five to 20 questions, all of which are associated with a specific topic. Question sets were selected from QBank that assessed whether students had mastered each topic in the content for each week in the course. Then the Moodle course management system was used to generate a unique homework assignment for each student each week.

Students were assigned weekly homework online through Moodle and given two attempts (*16*). Scores were determined by taking the higher score achieved of the two attempts. After submitting each attempt, students were given feedback that included links to pertinent pages within the online textbook. If a question had been answered incorrectly, the student could link directly from the homework grading screen to the online textbook to study text and examples related to the topic that was apparently not well understood. According to usage logs, students frequently made use of these links in the feedback while doing their weekly homework assignments. The course design assumes that students will often use the online text after missing questions on their first homework attempt.

The end-of-chapter questions from *Chemistry*, which were not part of the *JCE* QBank, were used in a different way. These questions were entered into Moodle and served as a collection of questions that students could use to review for examinations. The instructor selected appropriate questions and listed them for students. The students could then go to Moodle, answer the questions online, and obtain feedback regarding their answers. The use of assessment questions in these different ways illustrates an important difference between many online textbooks and ChemPaths: A great deal of effort has been expended to make ChemPaths a flexible and ubiquitous part of the general chemistry experience. ChemPaths is not just a textbook online; it is a new way of teaching a course where all aspects take advantage of instructional technology.

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Keeping a Living Textbook Healthy

As mentioned earlier, a student board was an integral part of both courses using the online textbook. Weekly meetings with interested, volunteer students allowed the instructor to modify the structure of the textbook, homework, and lecture to remove any unforeseen obstacles students may have had in adapting to cohesive online learning materials. Minor modifications were made at the request of the students throughout the first course that used the online textbook. The pages that introduced the reading for each date were updated to outline the reading, rather than just list the topics. The table of contents in the left side-bar was made more complete. Minor typographic errors were fixed and the class notified of any substantial changes.

The most important change was driven both by comments from the student board and the end-of-semester survey. A tutorial quiz was required of all students at the beginning of the second course in which the online textbook was used. This tutorial quiz forced students to perform a few basic tasks using the online textbook to familiarize them with its navigation and features. For instance, a number of students stated that they were frustrated with not having a search function—even though there is a search bar located at the top of every page. Thus, in the second use (and all subsequent uses) of the online textbook, one quiz question asked students to search for a phrase in order to complete a sentence, thereby insuring that they could do a search.

Diigo bookmarking and highlighting was not always used by students who could have benefitted from its use. In an end-of-course survey, some students commented that they missed being able to write on textbook pages and highlight text. This was a cause of concern, because Diigo was intended to serve those functions. At student board meetings, the students who used Diigo shared their success with the other students; many students used the Diigo tools successfully but many others did not.

In subsequent uses of the online textbook, the instructor may institute an assignment specifically designed to teach students how to use Diigo, because it is a powerful tool for annotation and communication. A similar situation is the use of a spreadsheet for data analysis; initially such use was optional for students, but eventually using a spreadsheet was deemed to be part of the curriculum and became a required assignment. Recently, Diigo has implemented an educator's account that allows creation of student accounts with higher privacy settings (http://www.diigo.com/education), and in the future this may be used so that students themselves do not have to agree to terms of use for a third-party software.

Students' preferences regarding use of notecards, highlighters, notebooks, and printed textbooks versus having their computer manage most of their studying tools are quite varied. The next section explores a little of what this means for students using today's online tools—and for their teachers.

Cultural Crossroads

The time we live in is a cultural crossroads. In the past four years of teaching, alone, some students have requested to have lecture materials entirely online for

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ease of access, while others begrudgingly agree to check their e-mail at most once every few days. Comfort level with electronic media seems to be a very important factor in how students will react to online learning materials. Before asking whether someone would use an online textbook, it may be more insightful to ask how he or she gets his or her daily news. In preliminary feedback from the courses using ChemPaths, there have been many contradictory responses, such as "I could find sections to study much easier with the online text" and "I can just find things easier with a physical textbook."

It is helpful for an instructor to know where students are likely to study and the availability of Internet access at those locations. If a student may want to use their textbook during lab then the instructor should make sure that students have access to a personal smart-phone or a wireless connection in the laboratory. A general poll of two semesters of students at UW-Madison who used the ChemPaths Web site gives some indication of where students use their online textbook. As expected, most students (over 95%) use their online textbook at home or in their dormitory. There are other locations on and around campus that students have accessed their online textbook, as seen in Figure 4.

Feelings regarding availability and comfort are most likely at a tipping point. Some students felt that the online textbook was more accessible, as it did not require carrying around the book or even a laptop. Others, however, said that they disliked the fact that they could only access the textbook when connected to the Internet. As the number of college students owning small, portable Web-accessible devices increases, and wireless connectivity expands, we expect that accessibility will become less of an issue. Anecdotal reports from teaching assistants indicated that some students used their iPhones to access their online textbook in lab, where many students do not typically bring their textbook.

Until this tipping point is passed, it will continue to be important to gauge students' level of comfort with and accessibility to the Internet in each specific course or institution before switching to an online-only textbook substitute. Different groups of students may have quite different responses.

Accessibility

Although "accessibility" was just used to describe student access to the online textbook, it is important to recognize the other use of the word in Web design: the ability for *everyone* to have access to *all* of the information contained on a Web site. As educators, it is our responsibility to teach all of our students—not just those with good vision, hearing, or dexterity. Therefore, it is of critical importance that instructors and designers are aware of principles of Web accessibility. First and foremost, attempt to adhere to the World Wide Web Consortium (W3C) standards for HTML, CSS and Accessibility (*54*). These are strict standards, and will substantially increase development time, but they should not be neglected.

ChemPaths was built using open source packages that adhere to most W3C standards. This cuts down on development time considerably compared to homegrown coding. Most institutions of higher learning also have on-campus resources for educators and students. The University of Wisconsin–Madison

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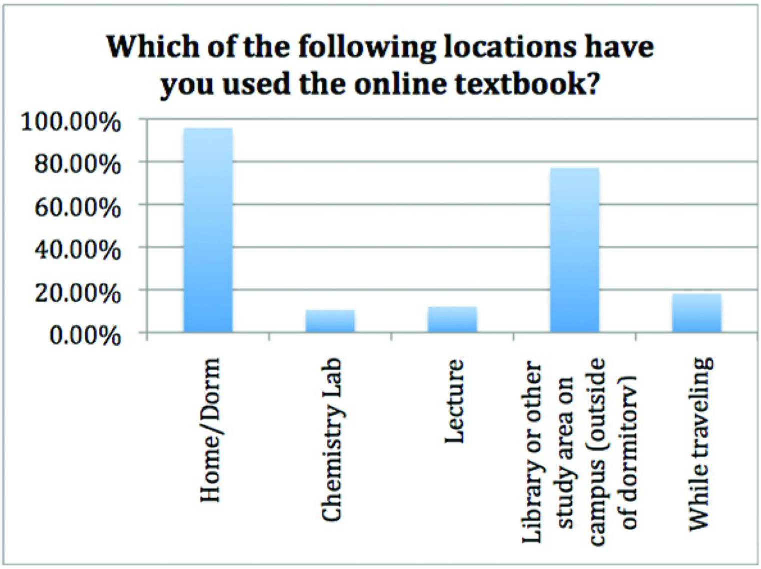

Figure 4. Results from a general survey of UW-Madison students in Chem 109H (80 students using the online textbook) and Chem 104 (180 students using the online textbook voluntarily of over 300 total).

Trace Center has many excellent tools and their Web site has links to development resources (*55*). Their on-campus seminars were of great value while building ChemPaths. The developers have built ChemPaths in such a way that it is widely accessible currently, and the chosen platform is streamlined to be fully accessible by year’s end.

Some items of concern that may surprise novice developers follow.

- Animations and videos should be described and/or narrated in text where a fully-able student would normally be expected to view the animation or video. Be descriptive. Using colors to describe objects to the those with impaired vision is not a slight; such students will find it helpful to have all the information available to a sighted person.
- When using interactive windows, be sure that there is an option to learn the same material in a text-based method.
- Find someone who can test sites using a screen reader.
- Be aware of the fact that HTML-tables get read from left to right in a screen reader. Thus, if data should be read in columns in order to make sense, use CSS to build the tables column by column.
- Avoid flashes of light and rapid motion in animations unless necessary. These can trigger seizures in portions of the population and are frequently not actually necessary.
- When possible, be able to print all text in pdf format. Resources for the blind are very adept at interpreting pdf files.

Once again, these are simply notable concerns and not an exhaustive list. Contacting a group of skilled professionals in testing for accessibility is invaluable.

Conclusion

Traditional, printed textbooks are the result of a long evolution of pedagogical design that sets them apart from mere collections of chemical facts, formulas, data tables, and encyclopedic information. Their authors, together with feedback from teachers/users, have carefully crafted textbooks to help students learn to solve problems and understand the chemical world. Both teachers and students are familiar with textbook design and are facile in its use. Nevertheless, as more and more proven pedagogical tools become electronic in nature (videos/animations (*37*, *49*, *50*, *56*), and 3-D molecular structures (*37*, *38*, *57*, *58*)), textbooks that utilize few of these tools in an integrated architecture become less desirable. As this chapter has shown, a great many new design decisions are enabled—and required—in the digital medium. Therefore, we encourage instructors and course designers to approach the era of the digital book with the understanding that *how* a book is designed—not just its content—is of fundamental pedagogical concern and can be changed.

Design Considerations

At this stage of development, there is no clear consensus on how to design an online textbook. Therefore we can only suggest what a designer ought to consider and how a designer ought to be guided. We do not feel competent to provide a how-to guide, but in this chapter we have described how we thought about the problem and what the outcomes of that thought were.

In the design of ChemPaths and in using ChemPaths to build two courses, we have been guided by important ideas in reviews by Wu and Shah (*7*) and by Yang (*34*). Both papers list features of a successful learning system. Wu and Shah are chemical educators investigating visuospatial thinking, whereas Yang is defining the synergy between hypermedia and constructivist theory. The original reviews provide detailed descriptions of terminology, but here we attempt to distil them to a concise list of considerations for developing an online portal along with the major headings from this chapter.

These considerations are collected in three overarching groupings: content, architecture, and pedagogy. One could argue that pedagogy should be employed in, and is inextricably intertwined with, development of both content and architecture. Indeed, no feature of a learning system is solely pedagogical. Nevertheless, we keep the pedagogy group explicit, because it helps to delineate the other features. The relationships are summarized as a Venn Diagram in Figure 5.

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Questions To Guide Design

Wu and Shah's guidelines were applied to smaller learning modules than an entire online textbook; however, our design guidelines for hypertext structure mirror their underlying motivation. Dillon *et al.* describe the landscape of hypertext documents as being a semantic space. Learners build a map, not unlike the way we convey physical space by use of landmarks and models (*4*). Thus, we propose a broader definition of the visuospatial guidelines of Wu and Shah, incorporating language from the realm of hypertext:

1. Provide multiple representations and descriptions of concepts.
2. Make linked referential connections visible among descriptions as well as among concepts.
3. Present the dynamic and interactive nature of chemical phenomena as well as the interlinked nature of chemical knowledge itself.
4. Promote the transformation between 2-D and 3-D.
5. Reduce cognitive load by making information explicit and integrated; likewise, make navigation focused.

With the exception of guideline four, each of these design criteria applies equally well to development of visuospatial thinking and semantic spatial thinking. We have described how ChemPaths has been built to incorporate each of these design guidelines within each of these areas.

- Architecture of site
- Layout of pages
- Assessment
- Interaction

Table I consists of 20 questions for developers of online textbooks, categorized according to these two lists of goals and design areas. It is our hope that these questions can guide design choices for future textbook substitutes, or inform decisions about whether to use other electronic resources within a course.

Each question in Table I has been addressed within this chapter as part of our description of the development of ChemPaths. Our consideration of these issues helped us to create a useful alternative to a traditional, printed textbook. ChemPaths truly offers an online textbook (learning portal) that is much more than just a book online.

In Enhancing Learning with Online Resources, Social Networking, and Digital Libraries; Belford, R., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2010.

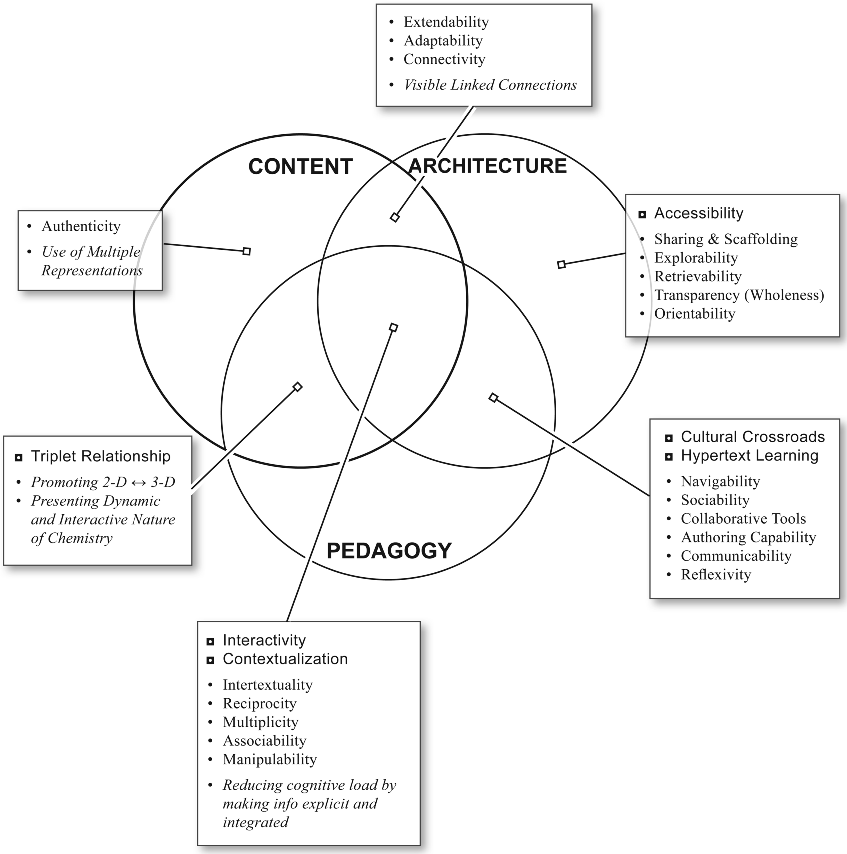
Extendability
Adaptability
Connectivity
Visible Linked Connections
CONTENT
ARCHITECTURE
PEDAGOGY
Authenticity
Use of Multiple Representations
Accessibility
Sharing & Scaffolding
Explorability
Retrievability
Transparency (Wholeness)
Orientability
Triplet Relationship
Promoting 2-D ↔ 3-D
Presenting Dynamic and Interactive Nature of Chemistry
Cultural Crossroads
Hypertext Learning
Navigability
Sociability
Collaborative Tools
Authoring Capability
Communicability
Reflexivity
Interactivity
Contextualization
Intertextuality
Reciprocity
Multiplicity
Associability
Manipulability
Reducing cognitive load by making info explicit and integrated

Figure 5. Mapping of key concepts and terms. Selected headings from this chapter can be found in a larger sans serif font with darker bullets. Functionalities from the review by Yang (34) and guidelines from the review by Wu & Shah (7) are shown in normal and italic serif fonts, respectively.

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Table I. Twenty questions for developers of online textbook replacements

	Provide multiple representations and descriptions of concepts	***Make linked referential connections visible both between descriptions as well as between concepts***	***Present the dynamic and interactive nature of chemical phenomena as well as the interlinked nature of chemical knowledge***	***Promote the transformation between 2-D and 3-D***	***Reduce cognitive load by making information explicit and integrated; likewise make the navigation focused***
Architecture	Are various contexts for a chemical principle available and clearly linked?	Does the navigation reinforce the proper schema for learners?	Are topics linked in a semantically relevant way to emphasize cohesion in the curriculum?	Do similar 2-D and 3-D representations exist for all linked contextual examples?	How easy is it for a student to get lost, or confined?
Layout	Is the use of text and multimedia cohesive within a topic?	Are connections visible and described within the text?	Is each chemical phenomenon described using all three levels of representation?	Are both 2-D and 3-D depictions available embedded in close proximity?	Is the layout simple enough to engender immediate appreciation for the topic while still enabling exploration?
Assessment	Are various assessment questions offered with multiple representations and/or contexts?	Does the assessment test understanding of the connections between representations and contexts?	Does the assessment require knowledge of the submicroscopic level of understanding?	Does the assessment require understanding the transformation between 2-D and 3-D?	Is the assessment tool stand-alone, or does it integrate into the learning material?
Interaction	Can students & instructors manipulate, control, or edit multiple representations?	Does the instructor reinforce the conceptual links and the representations within the text?	Can students easily navigate transition between linked representations and topcs?	Can students manipulate 3-D structures and/or are they able to build and edit their own structures?	Can students quickly acclimate to the navigation or interactive tools?

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Chapter 16

Building an Online Teaching Community

An Evolving Tale of Communication, Collaboration, and Chemistry

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The Interactive Online Network of Inorganic Chemists (IONiC) has grown from a small group of faculty to a national and international network focused on improving inorganic chemistry learning. IONiC's vision is to create a community of teachers and learners who *make teaching visible* using social networking tools to share, discuss, test, and assess their teaching methods. The features that have allowed the IONiC community to develop and grow and IONiC's vision for the future are described. It is likely that the lessons learned apply to other groups seeking to develop professional communities through social networking.

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We never set out to build an online community. The Interactive Online Network of Inorganic Chemists (IONiC) (*1*) and its digital home (the Virtual Inorganic Pedagogical Electronic Resource, VIPEr) (*2*) evolved from a faculty development initiative that brought together a group of inorganic chemists for a series of discussions, seminars, and brainstorming sessions to develop plans for modernizing the inorganic course and laboratory curriculum at our home institutions. A decade ago, this beginning might have been an end unto itself, or might have led to continued conversations in person at meetings. We might have shared some teaching materials and ideas by email. Instead, our collaboration began during the time when the social Web was blossoming, and both our collaboration and the results of our project have benefited greatly from the new ways of collaboration that the new technologies have enabled.

In the past decade there have been significant changes in technology and a transition from "Web 1.0"−online publishing—to "Web 2.0"−active online participation (*3*). Easier to use and lower cost videoconferencing and workflow technologies have made collaboration with geographically separated colleagues routine. The result is that we have had a much richer and broader conversation than we initially envisioned. The Internet provided us with a venue to both share materials and comment on and collectively improve them. Web-based communication technologies have allowed us to develop an online community that has become a hub for the discussion of teaching and learning of inorganic chemistry.

In this chapter, we will present the history of the development of IONiC—from a group of committed faculty to a network with broad national and international participation. We will highlight the features that we believe helped the initial community to develop as well as those that have allowed the community to spread beyond the initial developers. Finally, we will present our thinking about what we need to do in order to continue to grow and to increase participation in this community and others like it. Our community has worked to improve learning by making the process of our own teaching *visible*. Through iterative improvements in teaching materials and methods, we can learn from each other and improve student learning in all of our classes.

Why Did We Create an Online Community? The Development of the "Small Community" and a Community Home

The Leadership Council (LC) of IONiC is a very unusual community, both in composition and in how we interact with one another to accomplish our goals. It has eleven members—one technologist, one science librarian, and nine inorganic chemists. The LC has no formal leadership structure, geographically spans the United States, and its members range in academic rank from Assistant to Full Professors. We convene online weekly to carry out the business of IONiC and plan for the future of teaching and learning in inorganic chemistry. We are clearly a professional group, with grants, publications, presentations, and an award to our credit, and yet Donna Sundre, an assessment expert who has been interviewing the group for two years, has stressed the incredible personal rewards that we have reported, and the strong personal ties that we have built. The LC, in our persistent chat window on Skype (*4*), mixes discussions about child rearing, band gap theory, the group's Web site, recipes, an amusing Web link, and a video on social media—all in the course of a morning. There is a sense of close personal relationships that link us together; we are there for each other. For example, when one member was felled by personal circumstances toward the end of a semester, the group leapt to action and wrote her inorganic chemistry final exam.

Whether this is an example of the personal power of professional ties or the professional power of personal ties is both unanswerable and irrelevant. John Seeley Brown has spoken of how the Internet causes us to blend three personae of learning online: Knowing Human, Making Human, and Playing Human (*5*, *6*). Members of the LC interact daily, if not hourly, via online chat, in which we exchange knowledge, help one another create teaching materials, and manage to make it all feel like play. We engage in a mode of interaction that we call "Visible Teaching," (*7*) in which we share with one another our daily ideas, successes and failures related to teaching, but also collaboratively work to improve one another's courses. It is *this*, above all, that we think has transformed our approach to teaching inorganic chemistry, and that we wish to share with others. Of course, such a community did not develop overnight, or without the right environment in which these personal and professional ties could grow. As we look to the future, our goal is to help others—both in the community of IONiC and in the wider chemistry community—build the types of environments where their own small communities can grow.

IONiC was born in an Atlanta airport hotel meeting room during a gathering of participants in the Inorganic Chemistry Curricular Initiative (IC$_2$I). In 2006, the Mellon Foundation funded this effort to bring together six inorganic chemistry faculty members at Primarily Undergraduate Institutions (PUIs) for face-to-face networking in a series of three two-day seminars. One of the participants had previously met Kenny Morrell, Professor of Classics at Rhodes College and one of the founders of the *Sunoikisis* project. Sunoikisis (*8*) is an online collaborative learning environment in Classics, originally part of the Associated Colleges of the South and now available to all members of the National Institute for Technology and Liberal Education (NITLE) (*9*). We invited him to our first IC$_2$I meeting as a consultant, both to describe *Sunoikisis* and to help us envision what our own future collaboration might look like. One point impressed upon our group was the importance and excitement of doing collaborative work and the reinvigoration and community provided to participating faculty. After hearing his presentation, we were inspired to develop an online collaborative initiative for teaching inorganic chemistry. Inorganic chemistry is an especially good match for this type of collaboration, as the field is extremely broad with deep specialization of individuals in very different subfields. There is usually only one inorganic chemist at any given PUI, and he or she has limited ability to collaborate or interact with other inorganic chemists on a regular basis, especially in the sense of "passing in the hallway" informal contacts that are so important.

At a subsequent meeting, we met with Rebecca Davis and Michael Nanfito of NITLE and Ethan Benatan of Reed College, all leaders in educational technology, to develop our thinking about the form that an online community for inorganic

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chemists might take. For the chemists, this was a crucial first introduction to the ideas of the participatory Web, and as a result we teamed up with Benatan to design a Web site that would be a social, collaborative, evolving virtual library to share examples of course materials, curricular innovation, and best practices in teaching inorganic chemistry. We named the Web site VIPEr, the Virtual Inorganic Pedagogical Electronic Resource, Figure 1 (*2*).

From its inception, VIPEr was designed to be more than a repository—it was conceived as a platform to facilitate the sharing of materials for teaching inorganic chemistry and more importantly as a place where inorganic chemists could come to discuss teaching and research. The repository aspects of VIPEr were modeled after the *Analytical Sciences Digital Library* (*10*), the geosciences' *Starting Point* Web site (*11*), and Physical Chemistry On-Line (PCOL) (*12*). Although they are resources for much larger communities, the Multimedia Educational Resource for Learning and Online Teaching (MERLOT) (*13*), the National Science Digital Library (NSDL) (*14*), and the Chemical Education Digital Library (ChemEd DL) (*15*), were also inspirational. However, we were most influenced by a small organic chemistry Web site, *Not Voodoo* (*16*), an early example of the participatory Web. It demonstrated how the participatory Web could facilitate discussion and interactivity in a group of people with an interest in organic laboratory technique. *Not Voodoo* focused on the needs of a specific community, and provided a home for their conversations. We almost immediately embraced a Web 2.0 model to create a site where a community of inorganic chemists could take root, interacting through forums and discussion threads on learning objects. Throughout the project, our focus has been on the people and the conversation—the creation of a Web 2.0 community rather than a Web 1.0 resource.

The members of the LC benefited from the knowledge of key mentors during the early stages of this project. We also "learned by doing," and it is these lessons that we wish to describe.

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How Do You Create an Online Community? Lessons Learned from the Development of IONiC and VIPEr

The critical step for the development of IONiC, as is the case for most online communities, was bringing together a group of people to discuss something that interested them—in our case, teaching inorganic chemistry. Based on our experience and what we have observed in other online communities, we believe that there are some generalizable and transferable lessons about forming a virtual community. That said, probably no statement about online communities can be truly universal.

There Must Be a Latent Need.

What drives individuals to band together and form a community? Certainly the specifics will depend on the group; however, there is a commonality in that the individuals must believe that they will benefit from participation. They see the goals of the community as fulfilling a latent need or as a way to fill a specific niche in their lives. In other words, individuals will form a group if they believe they will receive some kind of personal benefit from the arrangement.

For the members of the IONiC Leadership Council, this need derived from our roles as inorganic chemistry faculty members at PUIs. The field of inorganic chemistry is one of the broadest in chemistry, covering the entire Periodic Table of the Elements, and is heavily specialized into subdisciplines. For inorganic faculty with diverse teaching loads and deep yet narrow training within a subdiscipline, curricular innovation faces considerable barriers. Since there is no "standard" inorganic course, either in terms of course level or content covered, deciding what topics to teach and at what level is challenging. This task becomes particularly formidable when faculty choose to incorporate topics outside of their comfort zone in lecture and laboratory courses. Collaboration with colleagues from different inorganic subfields is generally not possible within one's own department at a PUI due to small numbers, and geographical and professional isolation can make external collaborations difficult. Thus, the catalyst for the formation of our community was discovering that we were all trying to do the same things, dealing with the same problems, and realizing that we would all benefit from each other's expertise by banding together.

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There Has To Be a Broader Impact To Maintain Momentum.

The realization that there can be personal gain may be enough to initiate a community; however, in order to maintain momentum and sustain the community, there must be a broader reaching impact. Faculty members are pulled in many different directions. They must maintain an active research program, mentor students, and continually strive for excellence in teaching. In addition, they are expected to fulfill service obligations not only to their institution but also to their profession. With all of these demands on an individual's time, it would be very easy for the community to dissolve once it had at least, partially fulfilled the initial need. If the group is to persist, there must be some promise of a broader impact, reaching beyond the scope of the small community to serve to motivate and focus the group.

For the IONiC LC, this motivation came from realizing that some of the benefits we have received from this community could be spread to others through VIPEr, a Web site dedicated to teaching inorganic chemistry. We sought to enhance the inorganic chemistry classroom and laboratory experience for students and faculty members at many other institutions through the development and growth of the IONiC network. Participating in IONiC not only allows us to improve upon our own teaching, but also to serve the broader community.

Building Relationships Is Best Accomplished Face-to-Face.

The success of the community in accomplishing its goals is related to the strength of the ties between its members. While the personal gains and broader impact goals are critical for forming, focusing, and maintaining the group, there must also be personal connections among the members to achieve successful working relationships. Building personal rapport within the group makes completing difficult group tasks more enjoyable, while at the same time building a sense of mutual accountability among members.

Face-to-face meetings and personal connections were critical for forming the initial IONiC LC. We met several times, not only to flesh out ideas and goals, but also to build the relationships that would help to sustain the group. Technology and Web meetings were used to combat some of the geographical isolation, but it was the few face-to-face meetings each year that members really needed to recharge their batteries, reconnect with each other, build strong commitment to the project, and inspire them to keep moving forward. Over the course of this project, new members have been incorporated and cemented into the group through face-to-face project meetings. Whether it was reaching out to someone that an LC member knew from graduate school or meeting someone new at a professional conference, those personal connections have been key for getting new members to commit to joining the group and allowing them to become part of the community.

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There Must Be an Effective and Low Activation Energy Medium for Communication, Sharing, and Collaboration.

The emergence of Web 2.0 tools has made it possible for communities like the IONiC LC to accomplish its goals with the limited time and energy available for this project amidst competing demands. Early on, the LC met with technology specialists who demonstrated various tools available to the group. Since then, the LC has experimented with many different ways to communicate and collaborate.

File sharing for the initial grant writing efforts was carried out using Moodle (*17*), an educational classroom management system, hosted at DePauw. Moodle worked well as a repository for files, but poorly for real time editing. We now use two applications to share files. Documents that do not need to be polished, such as internal documents for the group, or early drafts of documents that benefit from simultaneous editing by several people, are created using Google Docs (*18*), while late-stage documents with significant formatting requirements, such as this book chapter, are edited using Central Desktop (*19*), a work-flow system. In Central Desktop, we cannot simultaneously edit a document, but instead check it out and check it back in. This helps manage the many versions generated in the final editing stage. In addition, it saves all versions of the document, so that text that has been edited out is not lost.

Weekly virtual meetings maintain communication and keep members on task in between our face-to-face meetings. We experimented using digital conference calls on Skype, but on more than one occasion had technical difficulties that led us to resort to "conference texting" instead of talking. Since then, we have progressed to videoconferencing on a weekly basis, first through Marratech (*20*), then Elluminate (*21*). The simple fact that we can see one another's faces on a weekly basis has an important psychological impact that ties the group together. Both Marratech and Elluminate allow simultaneous audio and video, although Elluminate's six video feed limit is not ideal because we have discovered the value in seeing everyone that is attending the meeting.

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Perhaps one of the most interesting technology uses that this group has found is a persistent chat in Skype. This feature has become the group's version of stopping to chat with a colleague in the hallway or around the coffee pot. By keeping a chat ongoing in Skype, group members can log on and communicate at any time. Sometimes the chat serves to answer questions about teaching, research, or a project the group is working on. Other times it serves a more informal purpose where members come to take a "coffee break," see what other people are up to, and just chat casually. Either way, knowing that the chat is there, members have a mechanism to communicate quickly, without clogging up each other's email inboxes. This chat window has replaced most of the more routine email communication within the group, though we still use email for important communications that no one in the group should miss. What we have learned is that our choices of the most effective Web 2.0 tools for collaboration change over time as the comfort level, needs, and personal ties in the LC evolve.

Commonality Brings a Group Together. Breadth Makes the Group Strong.

We like people like us. In the case of IONIC, this translated into a nucleus of faculty interested in sharing ideas about teaching and learning, enthusiastic about new technologies and their applications in teaching, and committed to the social network they have created. This small core dreamed and then created and cultivated an idea that has grown into a global network of like-minded educators.

While commonality brings a group together initially, it is the breadth of skills, interests, and ideas that makes a group strong. Initially, our definition of breadth encompassed only the sub-disciplines of inorganic chemistry. Most of us work at selective institutions that serve traditional residential undergraduate populations, but we have expanded our membership to include other types of institutions. Additionally, our professional interests beyond chemistry enhance our breadth. Drawing on our knowledge and expertise in fields spanning assessment, cognitive psychology, education, faculty development, history, and technology, we can approach problems from several different perspectives. We embrace and leverage the idiosyncrasies of our professional selves most *broadly* defined. Common interests and attitudes are a beginning, but we need a more diverse set of opinions—different schools, different students, different experiences—to really grow.

Not Too Big, Not Too Small

In order for our leadership group to function, the workload must be distributed in such a way that the tasks can be accomplished within the constraints of busy careers and families. For a group of individuals committed to the project and to each other, people are eager to volunteer for the projects they are most interested in, and willing to be volunteered for perhaps less interesting but still critical needs. There are conflicting issues with group size—the group needs to be big enough so that the work can be distributed, but paradoxically, the group needs to be small enough that it retains a sense of common purpose.

If the group is large enough, most of the work functions can be taken care of on a volunteer basis. For example, each semester seven LC members are assigned a weekly "Web site administration day" to activate new members, approve learning objects, and deal with any problems. It is critical for the success of the group that we deliberately keep the workload low, distributed, and weighted toward people with lighter semesters, sabbatical, or who are most dedicated to a given project. Importantly, by keeping the group size large enough to share the load, it allows for the occasional absence of one member of the LC for an extended period (heavy teaching semester, birth of a child, or medical emergency). Close and constant contact—regular check-ins—allows the group to anticipate some emerging needs before they arise.

The current group size of eleven active LC members has worked well for us. We have enough breadth in the sub-disciplines of inorganic chemistry that we can "cover" the content of the field. An unsurprising consequence of our large numbers is that it is almost impossible to schedule a weekly videoconference session that everyone can attend regularly. Growing the group significantly beyond its current size would almost certainly lead to a dilution of the close friendships that were (and are) essential for its function.

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There Must Be a Sense of Fun, Because Sustaining the Community Is More Important than Individual Tasks.

Here’s a good idea... take your regular 40-hour work-week (you’re already chuckling) and add 2-3 hours of Web site administrative duty, project planning, one extra conference call, and several hours of regular writing on top for no additional compensation. If we did not truly enjoy what we were doing, none of us would be doing it. The social aspect of *immediate contact* and *collaboration* with other inorganic chemists is something that most of us at a PUI thought we would never have. In IONIC, we have found a group of like-minded colleagues that share a love of inorganic chemistry, a geeky sense of humor, and a willingness to laugh at ourselves.

At our first face-to-face meeting, we decided that any acronyms for our group’s projects must be spelled with element symbols (and proceeded to come up with IONiC and VIPEr in a period of about a minute). We keep a running list of the particularly funny or outrageous things people say and turn them into a "quote quiz" for absent members of the LC. We have carried giant stuffed snakes through the streets of New Orleans and to our ACS Symposium. We have handed out VIPEr tattoos, and designed our own VIPEr "rock tour" t-shirts, and Buffs® emblazoned with our logo. Our project meetings have featured Diet Coke and Mentos bottle-rocket launchers, lots of home-cooked food and extra "fun days." As we put in long hours finishing up grant proposals, papers and book chapters in round-the-clock shifts, our Skype chat is filled with laughter, our own special emoticons, humorous Internet links, and evolving Wordle (*22*) tag clouds of the writing, Figure 2.

This camaraderie results in a commitment to the group and its goals far greater than was originally present when the group formed. In a small community, shared goals give rise to the community, but it is the ever-strengthening sense

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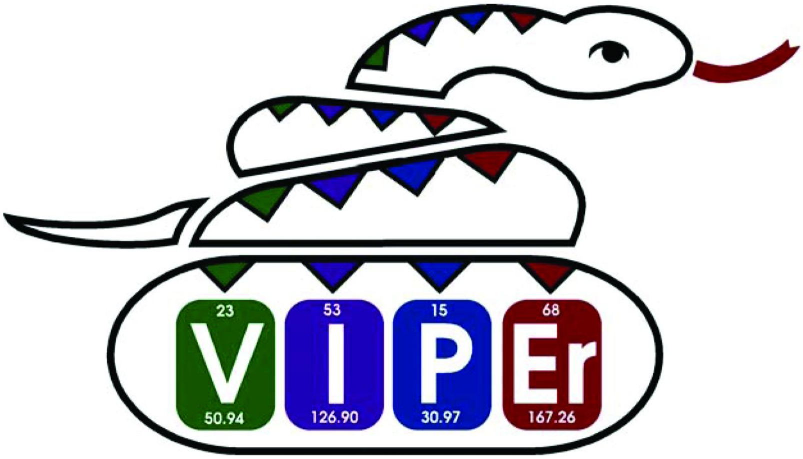

Figure 1. Logo for the Virtual Inorganic Pedagogical Electronic Resource

of connection that leads to continued forward momentum over time. Dedication and a sense of trust have made us very flexible and mutually supportive in our workflow. Each of us knows that if for some unanticipated reason we are unable to carry out a task that we were assigned (one that we may have even volunteered for), someone else will step in—something that has happened to each of us more than once. For us, the power of the community has been transformative.

IONiC: The Growth of a "Medium-Sized Community"

Expanding the community from a small group (the Leadership Council) to a larger one (the entire IONiC community) has relied on some of the same community building strategies that were used to develop the smaller leadership group. One key here has been forming a self-identified community where participation is rewarded, both in social and more tangible terms. In order to build and grow the IONiC community, we have pursued both on-line and face-to-face approaches: Web 2.0 features of the VIPEr Web site, regular e-mail communications to our users, publications, presentations targeting new participants at local/regional meetings, a regular presence at the national American Chemical Society meeting, hosting an annual research symposium, and various social events.

The VIPEr Web site itself provides a powerful way for the community to interact and grow. There are a number of Web 2.0 features on the site, including forums, commenting on learning objects, ratings, and polls, and these encourage site members to move from browsing and downloading learning objects to participation at a variety of "commitment" levels. There are many visits to the site by people who discover VIPEr through search engines (ca. 50,000 visits in the last year). To grow and sustain the IONiC community, however, we need to help this group of casual users see the individual and community benefits in moving from passively downloading materials from the site to significant participation. While at this point, members of the LC are the largest contributors to VIPEr, we

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are seeing an increasing number of posts from members outside of the LC; as of November 2009, 25% of the forum posts were from non-LC members. As our community has grown, we have seen an increase in overall site traffic and participation, but because of the wide daily fluctuations in viewership, we cannot correlate these increases to any particular event.

We keep in touch with the Web site community and help our users begin to take a more active role by sending periodic e-mails to our user list. Approximately quarterly, we announce updates to the VIPEr site, solicit feedback and participation in occasional surveys, and remind users, especially near the beginning of each semester, of the resources available on VIPEr.

Last year, we began a regular column in the *Journal of Chemical Education* (*23*). As we highlight teaching materials around a particular theme, we have contacted our users to solicit new learning objects that match the column topic and encourage rating and commenting on those learning objects chosen for the column. The possibility of a learning object being submitted for publication in JCE offers a readily recognizable "reward" for participation in the on-line community, encourages development of exemplary learning objects, and models the type of "Visible Teaching" that we hope becomes a natural part of all learning objects on the site.

We have focused on expanding knowledge of and participation in the IONiC community beyond those already registered on the site. One way for people to engage with each other in a community is through on-line publications such as CONFCHEM (*24*) and the Academic Commons (*25*). While the articles we have contributed to these sources are static documents, ongoing discussion is promoted through listservs (in the case of CONFCHEM) or comment threads (in Academic Commons). To date, the amount of discussion generated by either publication has been small, but it represents a nascent attempt at asynchronous conversation and has introduced our community to a broader audience.

The development of an annual ACS symposium was a direct result of our real need to provide face-to-face meetings for current and potential users of the VIPEr resource. Face-to-face meetings have been crucial to deepening community ties within the LC, and the same can be said about our broader user community. We have therefore been hosting a symposium at the spring national meeting of the ACS entitled "Undergraduate Research at the Frontiers of Inorganic Chemistry." At each of the past three spring ACS meetings, this symposium has provided a platform to get to know members of the community. At the first of these, the New Orleans ACS meeting in 2008, the initial VIPEr site was unveiled to the larger community. The response to the sense of fun at the unveiling was immediate—two of the speakers who are NOT members of the LC spontaneously chose to give their talks wearing our signature stuffed snakes. Casual conversations afterward focused on the previous lack of a community for inorganic chemistry teachers, echoing some of the reasons for the LC's founding. At the 2009 and 2010 spring ACS meetings, we again conducted symposia, allowing community members a chance to learn about each other's research, develop possible collaborations, and talk about the realities of being a teacher/scholar at an undergraduate institution. This ongoing symposium provides a standing mechanism for face-to-face meetings—a priority for the continued growth and development of the IONIC community.

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Figure 2. Wordle tag cloud of this chapter. Since word sizes correspond to word frequency, the wordle allows you to instantly see the main ideas in a piece of writing. This wordle shows how community is the central tenet of this article; community is at the heart of IONiC and Web 2.0.

In conjunction with each of these last two symposia, we have also organized social events. These well-attended gatherings help faculty meet in a more informal setting. Fostering these relationships help members feel more connected to the community, breaks down the barriers of anonymity, and convinces a new member to subsequently share his or her teaching materials on VIPEr. At our first social, for example, one faculty member expressed that she was not comfortable enough to participate online until she met some of the community members face-to-face.

Regional gatherings also provide an important face-to-face opportunity for community members to convene, especially for faculty who do not regularly go to national meetings. Many of these regional meetings are focused around geographical communities of teachers (*e.g.* MACTLAC (*26*) and MAALACT (*27*)) making them perfect places both to disseminate the VIPEr project and to develop personal relationships among the attendees and users.

Reaching out to faculty at major research institutions and encouraging them to participate in VIPEr is also an important priority for us. We have begun a conversation with this audience by presenting our Web site at research conferences in our subfields (such as Gordon Conferences) and have highlighted the important contributions at the cutting edge of our field that these faculty can make to the site.

How Do You Broaden Participation in an Online Community? Growing IONiC to a Medium-Sized Community

While it may be difficult to say exactly how big our "medium-sized community" is, we have used several metrics to monitor the growth of IONiC. As of Spring 2010, the VIPEr Web site had over 500 registered users and over 300 of them are verified chemistry faculty members from around the world. We have had a total of 76 oral presentations and 137 poster presentations at our three spring ACS meeting symposia (2008-2010). There are over 180 learning objects on the site and about a quarter of them were contributed by members outside the Leadership Council. Considering that the LC's efforts have focused more on the design and implementation of the Web site and less on community building (although that is coming next), we consider IONiC to be a healthy, medium-sized online community.

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As with the small-sized community of the LC, there have been transferable lessons learned from IONiC's growth to a medium-sized community that may prove valuable to other projects hoping to grow beyond a core of dedicated early innovators.

Make Participation Easy

The VIPEr Web site serves as the hub for our medium-sized community of inorganic chemistry faculty, and our design philosophy is to be inviting, easy to use, flexible, and interactive. We have been deeply influenced by Steve Krug's *Don't Make Me Think!* (*28*, *29*), which has served to keep the site navigation simple and intuitive, Figure 3.

The site layout, design, and logo were created professionally in order to make the site as inviting and attractive as possible, while still reflecting the personality and humor of the LC. The role of Ethan Benatan, the educational technologist in the group, was vital to this collaboration, because he could translate our desires into language that was meaningful to the professional site designers, and translate their questions back to us such that we could make informed design decisions.

We wanted to encourage participation and interactivity from the beginning. Thus, the social tools of discussion forums, polls, and rating and commenting on learning objects were included and given prominent place. This is, again, a case where Benatan's knowledge of the social Web was fundamental to good design. The original conception of the Web site was a simple library or repository of teaching tools. Only through exposure to the ideas and tools of Web 2.0 and translations of these concepts to the language of chemistry educators could we conceive of the notion of the Web site as a participatory and interactive online community.

Another counterintuitive choice for most members of the LC was to make publication easy and make peer review a post-publication rather than a pre-publication process. While we have not left the posting of learning objects completely open—they must be "approved" by a LC member before publication—we have embraced the model of crowdsourcing (*30*). Users post learning objects and community members then carry out *post-publication* peer review by leaving comments about what worked (and what didn't) and suggesting further modifications or additions.

We are cognizant of the fact that posting a learning object to a non-peer-reviewed Web site does not "count" toward professional advancement in the same way as a traditional peer-reviewed publication. While we have worked with the *Journal of Chemical Education* to create the *JCE VIPEr* column as a peer reviewed outlet for exemplary learning objects, we still depend on faculty generosity and their desire to share their best teaching practices with others for most contributions to the site. We have found that the quality of submitted learning objects is very high, and we assume this comes from faculty's own sense of professional responsibility and from the fact that they are making their work public to a community of others who know them. The rewards of participation are less quantifiable: gratitude in the comments, feedback on the learning object, and the opportunity to become an active member in a supportive community of

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chemists with shared interests. As intangible as these types of rewards may seem, they are at the heart of what makes virtually every Web 2.0 endeavor successful (*31*).

Finally, unlike a traditional journal, accepting one learning object on a Web site does not mean rejecting another. We are not restricted by page space, so we can encourage the submission and linking of similar learning objects, rather than trying to limit the number of learning objects. Rating systems, comments, search terms, and keywords can be a better way for people to find what they want. Given students' varied learning styles and instructors' varied teaching practices, what is best for one person might be different for someone else.

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Model Behavior in a New Environment

Making a transition to Visible Teaching requires a change in the way we approach our craft. Faculty educated in a pre-Web 2.0 environment need help imagining how technology tools can fundamentally change the culture of teaching, making it more open and transparent and encouraging personal ties between practitioners. For chemists with little Web 2.0 experience, peer mentors who can walk them through the process of becoming citizens in this new world can be a powerful catalyst for change.

As we developed the Web site, wrote our grants, and planned the future of our project, we saw firsthand the benefits of the social Web in our own interactions. We, like many before us, discovered that the whole point of Web 2.0 technologies is to connect *people*—to teach each other to do things and improve our skills. Web 2.0 is about community, people, and participation. As we fumbled our way through initial refinements of learning objects we posted on the Web site, we began to think about how to help our users understand and make the most of the site's format and features. After Joanne Stewart introduced Wiggins and McTighe's concept of *Understanding by Design* (*32*) to the group, we built new fields (and descriptions of what we were looking for in those fields) into our learning object submission forms. These new fields encourage the inclusion of learning goals, outcomes, and assessment with a submitted learning object. Stewart also submitted a "5 Slides About" learning object on *Understanding by Design* in order to show potential authors what should be included in each of the fields (*33*). This particular learning object has been very popular, having been downloaded 541 times in the year since it was first posted (Jun 2009 - Jun 2010).

As we have improved our own understanding of the benefits of Web 2.0, we have focused on modeling the types of contributions that we hope to get from others. We have tested each other's learning objects, rated them, and posted comments on how we have adapted them to our own classrooms. We have had conversations about the learning object in the comment threads so that our community could see the benefits of these interactions. We post new forum discussion threads and answer posts of other community members. In moderating new learning objects that others submit, we have taken an active role, encouraging authors to follow our format and offering helpful suggestions on how to improve the materials. We remind our users about rating and commenting on learning objects, as well as submitting new objects, in periodic emails to our user

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community. LC members have reached out to possible new submitters, offering to walk them through the process. In-person workshops at regional and national meetings have also been a way to model and talk about the value of Web 2.0 interactions to new users.

Develop Plausible Promise for Your Users

Mirroring the experiences and requirements for growing and maintaining the LC, new community members need both a reason to come and a reason to stay. While a first visit to VIPEr may be the result of a random Google search for information on textbooks, a deliberate search for teaching materials, or a personal invitation by one of the community, users need a reason to return if the Web site is to grow as a community. We rely on the appeal of the Web site and the quality of the content to achieve this goal.

Still, if we are to convert users into active members of the community, the site and the group has to offer something more than content. We must expect that new members have all the same stressors and responsibilities that we in the LC have. For example, one member posted the following: "Help, I’m under assault," and described his concern about a department curriculum review leading to the possible demise of one of their two inorganic courses. Within a few hours he had received three thoughtful responses to bolster his arguments for keeping the course.

For some of our community, the opportunity to engage in conversation is enough, but if we want to deepen the conversation a bigger carrot is often required. We offer this through the opportunity to have one’s work recognized in the *Journal of Chemical Education* column and through sponsoring the ACS symposium, an opportunity for PUI faculty to have a research "home" in the vast ACS meeting program. Our initial solicitation for learning objects, with the plausible promise of consideration for publication in the *JCE VIPEr* column, yielded the submission of several learning objects from first-time contributors. Participation in workshops sponsored by IONiC also counts towards professional development in tenure and promotion at some institutions.

Expect Different Levels of Participation from Participants

A repository just needs users, but a community needs participants. The latter is a tougher sell for busy academics. Initially, we focused on cultivating new users, with the thought that if we could attract users, a significant number would become active participants. However, despite our success recruiting users, most contributions still come from the LC.

IONiC fits the definition of a "community of practice," from Lave and Wenger’s work on situated learning, in which learning involves a "deepening process of participation" (*34*). Lave and Wenger introduced the term "legitimate peripheral participants" to describe new community members who learn primarily through observation and the completion of simple tasks. The online world has traditionally called these "lurkers." Lurkers, however, has a pejorative connotation, whereas Lave and Wenger argue that legitimate peripheral participation is a

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necessary early stage of even the most active contributors. VIPEr statistics show the VIPEr site to be a typical Web-based community of practice in that there are a small number of core users—the LC—a slightly larger number of moderately active participants, and a very large number of legitimate peripheral participants who read the forums and download learning objects but do not actively contribute. The latter two groups form the "long tail," the large number of users who each contribute only a small amount, but when taken together, make up a significant impact (*35*).

It is important to 1) make sure this participation model can sustain the site, 2) provide multiple ways for the moderately active participants to engage more deeply with the community, and 3) find ways to increase the participation of the lurkers. We have thus far had some success encouraging lurkers to become more active members through face-to-face workshops at professional meetings. We have also been able to grow and sustain the site through the actions of the core users and the moderately active participants. The development of the community will be our primary emphasis over the next few years.

Build a Community Home that Looks Like a Home to the Community

One of the common criticisms we receive is "Why did you create yet another Web site when there are already well-developed resources out there like MERLOT that you could contribute to?" We agree that MERLOT, the ChemEd DL, the NSDL, and other sites have many great learning resources. But these resources do not provide the focus, the identity, and the home that we were looking for. It is the narrowness and focus of VIPEr and the shared practice of the participants that make it work for the inorganic chemistry community. It is the opportunity to post questions about inorganic research or teaching that will be answered by faculty who really understand that field. It is the opportunity to share humor that is likely only funny to other inorganic chemists. Who else really cares how "chalcogens" is pronounced or whether CH_2Cl_2 is called methylene chloride or DCM? Who else would name their site (and community) using acronyms that can be made up of element symbols from the Periodic Table?

Not only does the organization of the site reflect the way that inorganic chemists think about teaching inorganic chemistry, organized on the home page by subdisciplines like organometallic chemistry and bioinorganic chemistry (Figure 3), but it also reflects the LC's strong interest in active, engaging pedagogies. There are learning objects that emphasize in-class activities, reading the current literature to learn fundamental concepts, and even kinesthetic learning, such as *Catalytic Cycles and Artistry: Chalk Drawing 101* (*36*) and *Athletic Periodic Trends Review* (*37*). The site feels like home to faculty interested in improving inorganic chemistry learning.

Have an Overall Vision for the Community

Chemists like results. A group's vision is a concise statement of what it wants its results to be—of what success would look like. For IONiC, that vision is the movement of inorganic chemistry teaching from private to community spaces,

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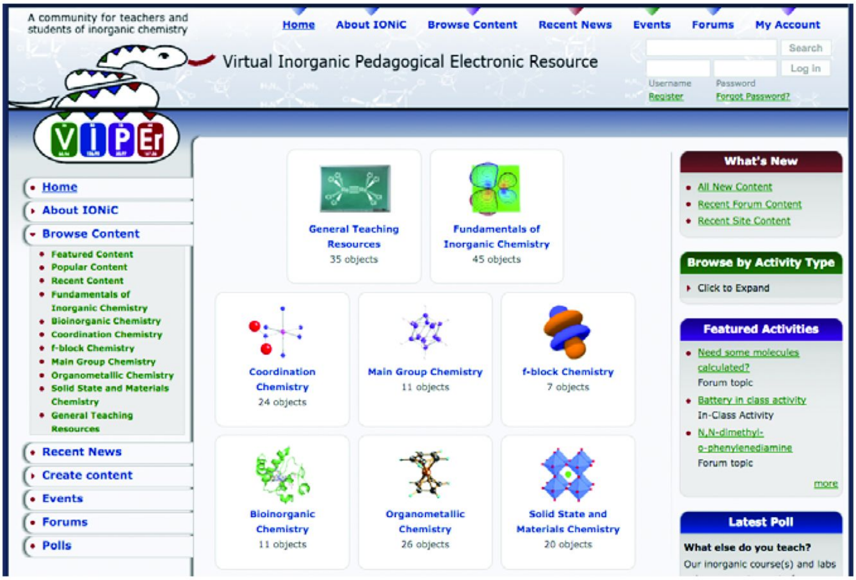
A community for teachers and students of inorganic chemistry
Home
About IONiC
Browse Content
Recent News
Events
Forums
My Account
Search
Log in
Username
Password
Register
Forgot Password?
Virtual Inorganic Pedagogical Electronic Resource
VIPEr
Home
About IONiC
Browse Content
Featured Content
Popular Content
Recent Content
Fundamentals of Inorganic Chemistry
Bioinorganic Chemistry
Coordination Chemistry
f-block Chemistry
Main Group Chemistry
Organometallic Chemistry
Solid State and Materials Chemistry
General Teaching Resources
Recent News
Create content
Events
Forums
Polls
General Teaching Resources
35 objects
Fundamentals of Inorganic Chemistry
45 objects
Coordination Chemistry
24 objects
Main Group Chemistry
11 objects
f-block Chemistry
7 objects
Bioinorganic Chemistry
11 objects
Organometallic Chemistry
26 objects
Solid State and Materials Chemistry
20 objects
What's New
All New Content
Recent Forum Content
Recent Site Content
Browse by Activity Type
Click to Expand
Featured Activities
Need some molecules calculated?
Forum topic
Battery in class activity
In-Class Activity
N,N-dimethyl-o-phenylenediamine
Forum topic
more
Latest Poll
What else do you teach?
Our inorganic course(s) and labs

Figure 3. The homepage of VIPEr. The Web site was designed to be accessible to inorganic chemistry educators by including traditional representations of the subfields of inorganic chemistry.

or "Visible Teaching." While a Web site that is simply a repository of lecture notes, in-class activities, and problem set questions would have some value, our online community aspires to widely promote the idea that the social aspects of collaboration and sharing in teaching can be of as much value as collaboration and sharing in research. By working collaboratively and iteratively to improve VIPEr's learning objects based on community suggestions and assessment results, we become better teachers and participate in a vision of Visible Teaching that has the potential for changing the culture of the academy.

Looking Ahead: Expanding the IONiC Community and Promoting Visible Teaching

When we began this project, our goal was personal—to improve the teaching of inorganic chemistry at our own institutions. As we have engaged in Visible Teaching, we have realized that there are enormous benefits that come from discussing our classroom practices and sharing our teaching materials. We believe the entire community can benefit from this mode of teaching. There is a large community of inorganic educators who have much to contribute to this discussion, and by leveraging the community, we can tap an enormous reservoir of distributed knowledge. However, large communities function in a very different way than small, or even medium sized, communities. Our latest challenge is to develop a plan of action to bring the benefits of small communities engaged in Visible Teaching to a much larger community. How do we go about community development? There is an enormous literature devoted to this topic that we are learning and applying to IONiC (*38–40*), and here we outline our next planned steps to achieve this goal.

Provide the Tools To Engage in Visible Teaching

Early in the project, we realized that we did not have some of the key skills that we needed to develop VIPEr and IONiC. None of us were experts in social networking technologies, nor did we initially recognize the importance of these technologies. We were not Web 2.0 denizens in our personal lives so we could not understand how these social tools would translate to our professional lives. We did not appreciate the participatory Web. The critical element for the development of IONiC as an online community was having mentors and collaborators who could teach us technology tools in the context of something we already understood—teaching inorganic chemistry. By learning these tools in context, we could see their professional value and impact. Future members of the IONiC community might also be unfamiliar with using social networking tools in a professional setting. Thus, it is critical that we mentor new community members in using these tools so that they can appreciate their role in Visible Teaching.

While we all care deeply about teaching and constantly strive to provide our students with the best possible learning environment, we are not experts on the literature of misconceptions, metacognition, and assessment; we are trained as PhD chemists, not as educational specialists. To ground our efforts in Visible Teaching within the context of what is known about student learning, a LC member knowledgeable in this area translated the principles of *Understanding by Design* (*32*) into concrete examples of structuring learning objectives and developing assessments that are accessible to chemists (*33*). Our understanding of assessment practice has been transformed because we have a model that directly applies to our area of expertise translated into the language of student learning. Once again, by developing expertise in a comfortable context, community members can learn and incorporate this tool into their teaching practice.

The first step to engage the broader community in a Visible Teaching model of pedagogical collaboration and innovation is to help a cohort of new users develop expertise in technology and assessment tools in context. The Great Lakes College Association (GLCA) members of the LC (Eppley, Stewart, and Watson) will take a step toward strengthening the IONiC community by hosting a workshop introducing chemists to Web-based collaboration tools and to VIPEr. In these workshops, participants will become familiar with technology tools that enhance Visible Teaching and Understanding by Design practices. They will learn how to use these tools to improve student learning in the context of the courses that they teach. We plan to extend this model to a larger audience with future funding.

Develop IONiC as a "Loose-Ties" Large Community Made Up of "Strong-Ties" Small Communities

While our vision of IONiC is a large community encompassing many inorganic educators, smaller communities have an advantage over larger

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communities because participants know each other well. Small groups with strong ties function better because everyone does their share of the work and reciprocity is both expected and enforced. Personal ties and civic-mindedness keep the group moving forward. However, any individual small community has limited reach. Thus, we envision the community moving forward as a whole made up of smaller communities with strong ties—groups of what we call IONiC Scholars. Each of these groups will initially be born out of extended face-to-face interactions in a workshop, and will be able to continue online as a cohesive community after the workshop is over.

We consider each strong-ties community as a cohort of IONiC Scholars. As the community founders, the LC are the first group of IONiC Scholars. Together, we have learned the technology tools needed to engage in Visible Teaching. Over the past three years, our relationship with technology and our understanding of the social Web and student learning have evolved, changing our teaching and conceptions of student learning. We have inadvertently engaged in our own faculty development plan! We envision GLCA workshop participants to be second cohort of IONiC Scholars and eventually hope to mentor additional cohorts. Once they learn the collaborative technology tools, they will be able to engage in Visible Teaching. As a semi-independently functioning small group, they will act as a support community for each other, participate in the larger VIPEr community, and help vision the future of IONiC. Not every group will evolve in the same way that we have, but we hope to lay the foundation so that each of these groups can become a strong-ties community with the tools to engage in scholarly work focused on inorganic education in whatever way their interests, strengths, and future developments in technology take them.

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Lower the Barriers to Participation

The Internet is changing how we communicate with the world. Previously, scientific communication has been confined by “Gutenberg economics”—the high cost of making information public (*41*). In this model, dissemination costs are high so it is necessary to erect barriers to control flow. The barrier, or filtering mechanism used in science, has been pre-publication peer review. Only things that have been vetted by community "experts" are published. We see this as a way of validating information, but it also is a way of restricting information. A barrier has been placed before dissemination.

We are products of the pre-publication peer-review system. To us, pre-publication peer-review defines the culture of science. This is a mechanism whereby we filter then publish. Once published, material is generally static. On the Web, a more dynamic mechanism is possible that is extremely effective in software development—publish than filter (*42*). The Internet is an ideal medium to convene scientists to discuss a piece of work. Part of this is familiar; it is the back and forth in which we participate at meetings. Since anyone can review or discuss a publication and provide suggestions for the author to increase the value of the contribution, the author can benefit from the ideas and criticisms of everyone interested in the paper. Frequently, the discussion is as valuable as the idea; the Internet allows both to be disseminated.

There is, however, a source of tension that arises by moving to this new model; in the publish then filter model, everyone can have a voice. This is an uncomfortable idea for scientists; we are used to information being controlled by experts. Yet non-experts span a breadth of disciplines; they can be complete neophytes or experts in other areas of chemistry, science, education, cognition, etc. Frequently, the non-expert often brings a valuable and different perspective to a problem that can provide the necessary insights to solve trivial or intractable problems (*30*).

Community openness is a constant source of tension between the technologists and chemists on the LC. The chemists want to restrict the conversation on VIPEr to experts—only people engaged in teaching and learning chemistry should be able to contribute learning objects and comments. We assume that there is more value in a learning object contributed by a faculty member than a first year undergraduate. This may well be the case, but not necessarily. The technologists argue for complete openness of VIPEr. Everyone should be able to contribute equally and the community will eventually assign value to contributions to VIPEr. The most important element for a community is participation. Filtering erects barriers to participation that are usually high enough to squelch a fledgling community. Controlling information limits the conversation. During this project, our educational technologist has encouraged us to move towards a model where we eliminate barriers to participation by letting anyone who conforms to the standards and ideals of the community participate. While this is an unfamiliar and uncomfortable idea to many of us, we are gradually moving along that path.

We have significantly lowered barriers. Anyone who registers on VIPEr can comment. Anyone who has faculty status can contribute in any way. We monitor for relevance rather than quality. However, we still have barriers in place. The LC defines what types of learning objects can be contributed; we define how they look. We have limited the development of learning objects to faculty (or students with the assistance of a faculty member). To be fully engaged, the entire community must define what makes a learning object and have the freedom to experiment. We have opted to use only asynchronous methods of communication on VIPEr, but to engage the community, we may need to incorporate real time communication tools like Twitter (*43*) feeds or chat rooms.

It is an exciting time to be involved in a project that bridges traditional publishing and an open publication model. A paradigm shift in publishing and peer-review seems imminent. Scholarship is shifting from "three people review it, once, prior to publication" to "a large number of people can potentially review it post-publication, in a process that never ends." The costs of dissemination have been greatly lowered—on the Web; everyone can be an information contributor, not just an information consumer. Eric Raymond says that the development of Linux needed to follow this model because no small group of reviewers could find the problems, but the whole community could: "Given enough eyeballs, all bugs are shallow" (*44*), meaning that with enough diverse talents and interests, every bug is easy and interesting for someone to fix. By moving the process of peer review to the other side of publication, it is easier for experts from many communities to contribute and make their views known. This may not be an easy

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Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ch016

transition for our community (*45*, *46*), but it is the one that will foster the spirit of collaboration

Conclusions

We began this adventure as a small group of faculty who were only vaguely aware of the possibilities of online communities. We are now seeing the transition of our community from this small group of initial builders to a wider user base. While we still have work to do in increasing participation from the larger community, we are already seeing the initial evolution from a site that mostly acts as a repository with a few forum posts by the Leadership Council to a site that showcases Visible Teaching and includes participation in forums and comments and posting of Learning Objects from community members. As we work to form additional small communities with close personal ties, provide faculty development in the concepts of Visible Teaching, a culture of assessment, and using Web 2.0 technologies, we anticipate the further evolution and hopefully growth of this community.

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Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ch016

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Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ch016

Subject Index

A

Accessibility and online textbook, 300
Access information, changes, 140
Animation
  chemistry education, 175
  design, 175
  education, tool, 168
  expert models, 169
  Jmol, 73*f*
  multimedia
    design and use, 167
    learning, 176
  visualization, 168
Ash canker, 269*f*
Assessment and student portal for learning, 298

B

Bazaars, 101
  and cathedral, 103
  science, 107
  third millennium, 106
Behaviorism and cognitive psychology research, 170
Bishop, Mark, 286
Black, Joseph, 286
Blogs, 54
Book online, 283
Boyle, Robert, 95
Broken market of textbooks, 271

C

Cambridge crystal database, 75*f*
Cathedrals, 101
  and bazaars, 104
ChemEd DL. *See* Chemical Education Digital Library
Chemical data online, resourcing, 26
Chemical education
  eBooks, 137
  open access journals, 136
  social networking, 7
Chemical Education Digital Library
  Models 360 site, 72*f*
  Periodic Table Live!, 72*f*
Chemical scholarship and changing environment, 129
Cheminformatics and education, 25
Chemistry
  ChemPRIME, 263
  didactics, 263
  education
    animation, 175
    21st century, 65
    Web-based molecular visualization, 65
  pedagogy, 263
  wikipedia, 79
ChemPaths
  contextualization, 289
  daily page, screenshot, 297*f*
  hypertext learning, 289
  interactivity, 218
  Learning to Meander, 287
  triplet relationship, 289
ChemPaths Student Portal, 283
ChemPRIME
  chemistry, 263
  curriculum, improved, 270
  eBooks, 271
  educational philosophy, 268
  exemplars, 267*f*, 268*f*, 269*f*, 270*f*
  general chemistry courses
    contributors and modifying pages, support, 278
    online quizzes, 278
    order of topics, 277
    project, 279
    sabotage-proof pages, 277
    University of Arkansas at Little Rock, activities, 278
    wikis, use, 276
  open books, 271
  pedagogy, improved, 274
  structure, 265
  textbooks, broken market, 271
  wiki text, 263
ChemSpider
  Google patents, 34*f*
  integrating structure-based resources, 23
  Internet, 28
  project prospect, 57
  proton NMR spectrum, 35*f*
  record, 33*f*
  spectral game, 35*f*
  Synthetic page, 34*f*
  Xanax, 33*f*, 34*f*

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Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ix002

CIMS. *See* Core ideas in molecular science
Cognitive psychology research
  behaviorism, 170
  cognitivism, 170
  guided-inquiry, 173
  situated learning, 170
Cognitive Tutoring Authoring Tools and behavior graph, 246*f*
Commerce and free resources disruption, 36
Constructivist Unifying Baccalaureate Epistemology system, 162*f*
Contextualization
  ChemPaths, 289
  context-based approaches, 291
  project, 287
Core ideas in molecular science, 238
Crystallography and inorganic chemistry, Web-based molecular visualization, 75
CTAT. *See* Cognitive Tutoring Authoring Tools
CUBE. *See* Constructivist Unifying Baccalaureate Epistemology
Cultural crossroads
  online textbook, 299
  University of Wisconsin–Madison students, 301*f*
Curriculum development projects
  CIMS, 238
  stoichiometry course, 238
  virtual lab collection, 237

D

3-D and 2-D molecular visualization and Cambridge crystal database, 75*f*
Data
  access and scientific literature, 134
  design, 196
Design
  principles and instruction online, 252
  textbook, online, 302
    key concepts and terms, mapping, 304*f*
    questions, 303, 305*t*
Didactics of chemistry, 263
Digital libraries
  creation, 12
  current status, 52
  instructional components, 238*t*
  learning, enhancing, 1
  online resources, disseminating, 12
  refining, 12
  storing, 12
Diigo and student portal for learning, 297
3-D molecular models and Web page, 67
DynamicBooks, 287

E

e^{2}Book, 149, 164*t*
eBooks. *See* Electronic-books
Education
  cheminformatics, 25
  e-Learning, 154
e-Knowledge, 149
e-Learning
  education, 154
  integrated, 149
  paradigms, 153
  terminology, 155*t*
  Web background-history, 151
Electronic-books, 154, 157
  chemical education, 137
  ChemPRIME, 271
  design issues, 178
  formats, 156
  IC2, 180*f*
  integrated learning environments, 149
  publishing formats, 157*t*
  readers, 156*f*
  technology, 156
  textbook online, 286
Emerging technologies
  Follett CafeScribe eBook, 163*f*
  integrated learning environments, 162
  McMillan DynamicBooks, 163*f*
e-Readers, 158
EX$_2$. *See* Explanations with examples system
Explanations with examples system, 242*f*
  instruction online, 240

F

FOAF. *See* Friends of a Friend
Follett CafeScribe eBook, 163*f*
Forms of collaboration and open chemistry, 132
Free resources disruption and commerce, 36
Friends of a Friend
  aggregation
    ChemSem, 53*f*
    group, 48*f*, 52*f*
    personal, 48*f*, 51*f*
    professional Web page, 53*f*

Downloaded by 89.163.34.136 on June 23, 2012 | http://pubs.acs.org
Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ix002

Downloaded by 89.163.34.136 on June 23, 2012 | http://pubs.acs.org
Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ix002

    - scientific profile, 52
    - scientist's molecules of interest, 51
    - Semantic Web vocabulary, 48
    - SemanticEye, 51*f*, 52*f*, 53*f*
    - single person, 53*f*
    - SPARQL, 49, 50

G

- General chemistry
  - ChemPRIME, 276
  - courses, 276
  - Web-based molecular visualization, 70
- Generic visualization structure, 160*f*
- Ghiacciaie in Florence, Italy, 267*f*
- Global society and knowledge, 95
- Google Jockey, 124
- Grade distributions and learning protocols, 183*f*
- Group FOAF of SemanticEye output, 52*f*

H

- Hasse diagram, 194*f*
- Hayek's knowledge problem, 103
- Hobbes, Thomas, 108
- Hypertext learning, 288
  - ChemPaths, 289
  - organization and pedagogy, 289

I

- IC2. *See* Inductive Concept Construction
- ILE. *See* Integrated Learning Environment
- Inductive Concept Construction
  - learning system
    - classroom, 181
    - eBook, 178, 180*f*
    - out-of-the-lecture hall cooperative learning, 181
    - survey, 182
- Information
  - collection
    - personalized information management system, 115
    - RSS, symbols, 118*f*
  - Google Jockey, 124
  - image delivery, 124
  - organization, 119
  - paradigm, new, 129
  - presentation and synthesis, 122
  - small packages, 123
  - Twitter, 123
  - wikis, 122
- Inorganic chemistry and Web-based molecular visualization, 70
- Inquiry learning processes, 173
- Instructional components and digital library, 238*t*
- Instruction online
  - components, 235
    - explanations, 240, 242*f*
    - moving classroom lectures online, 240
    - moving text online, 239
  - design principles
    - chemical and physical models, 255*f*
    - configurable simulation, 255
    - 3-D box use, 256*f*
    - domain, analyze and re-envision, 253
    - energy landscapes, 255*f*
    - modality, 252
    - population distributions and temperature, 256*f*
    - simulation, 256*f*
    - technology choice, 258
    - visualization components, 255
  - OLI flash based components, 245*f*
  - questions, 243
- Integrated learning environment
  - case analysis rubrics, 160*t*
  - CUBE system, 162*f*
  - eBooks to e^2Books, 149
  - e-Learning 3.0 to e-Knowledge, 149
  - exam performance comparison, 162*f*
  - knowledge repository, 159
  - quantitative analysis, 161
  - research, 162
  - semantic framework, 161*t*
- Interactive Online Network of Inorganic Chemists
  - expanding, online teaching community, 324
  - medium-sized community, 317, 319
  - online teaching community, 312
  - Web 2.0, 319*f*
- Interactivity
  - ChemPaths, 289
  - online course design, 218
  - theoretical framework, 291
- Internet and ChemSpider, 23, 28
- IONiC. *See* Interactive Online Network of Inorganic Chemists

J

Java molecular editor
  2-D to 3-D conversion, 74*f*
  Jmol, 74*f*
Jmol
  animation, 73*f*
  applets, molecular geometries, 70*f*
  Java molecular editor, 74*f*
Jmol Molecular Visualization Project
  animation, 73*f*
  3-D molecule model, 67*f*
  Java molecular editor, 74*f*
  Jmol applets, 70*f*
  structure file formats, 68*t*
Journal articles
  project prospect, 57
  SemanticEye, 45, 47*f*

K

Knowledge
  global society, 110
  map, 194*f*, 196
    application functional component workflow, 197*f*
    assessor, 196
    constructor, 201
    correlation measure, 199
    directed dependency measure, 198
    order distance metric, 198
    organic chemistry, 191, 205*f*, 206*f*
    weight scaling, 200
  power law distribution, 105*f*
  space theory and applications, 193
    organic chemistry, 195
  state model, 200

L

Laplace, Pierre-Simon, 267*f*
Lavoisier, Antoine, 267*f*
Learning
  enhancing
    digital libraries, 1
    online resources, 1
    social networking, 1
  instructional philosophies, 153
  objectives, 150
  order, 199*s*
  protocols and grade distributions, 183*f*
  theories, 167
Lecture and student portal for learning, 181

M

Macmillan, 287
Magma and ChemPRIME exemplar, 269*f*
Mashups, 57
McMillan DynamicBooks, 163*f*
Medium-sized community and IONiC, 317, 319
Multimedia
  learning, 176
  pedagogy and learning theory, 167

N

Nanoscience
  teachers
    course features and descriptions, 219*t*
    Spring 2007, screenshot, 220*f*
  topics, 214*t*

O

OLI flash based components
  tutor, 245*f*
  user-interface panel, 245*f*
Online chemical data, 26
Online chemistry resources, future, 33
Online course
  content
    accuracy and relevance, 214
    choose, 213
    copyright considerations, 216
    course management system, 217
    laboratory and hands-on experience, 215
    layout, 217
    nanoscience topics, 214*t*
    Web content, 215
  design, 211
  interactivity, 218
    content, 225
    instructor, 219
    peers, 222
Online instruction, 235
Online journals, 130
Online practice questions, 243
  authoring systems, 244
  CTAT system and behavior graph, 246*f*
  empirical formula tutor, 247*f*

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Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ix002

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Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ix002

  molecular level visualization and simulations, 251
    progress of reaction, 252*f*
  OLI flash based components, 245*f*
  virtual laboratory, 247, 250*f*
Online resources
  current status, 52
  learning, enhancing, 1
  open resources, 4
  open science, 4
  pedagogy and curriculum, 9
Online teaching community
  community home, 310
  create, 310, 312
  IONiC, 312
    expanding, 324
    visible teaching, 324
  need, 312
  participation, broaden, 319
  small community, 310
  VIPEr, 312, 313
  Wordle tag cloud, 319*f*
Online textbook, 283
Open access journals and chemical education, 136
Open books, 271
Open chemistry and forms of collaboration, 132
Open resources, 4
Open science, 4
Order distance distributions, 199*t*, 201*f*
Order distance metric, 198
ORDVAC 1, 152*f*
Organic chemistry
  knowledge
    map, 191, 205*f*, 206*f*
    space, 195
  Web-based molecular visualization, 71

P

Pedagogy
  ChemPRIME, 274
  general chemistry course, 263
  multimedia, 167
  online resources, 9
Personalized information management system
  creating and using, 115
  Google Jockey, 124
  information
    collection, 117
    image delivery, 124
    organization, 119
    presentation and synthesis, 122
    small packages, 123
  RSS, 117
  social tagging, 119
  Twitter, 123
  wikis, 122
Podcast, 56
Power law distribution and knowledge, 105*f*
Problem success predictor, 196
Project prospect
  ChemSpider, 57
  journal articles, 57
Pseudomonas syringae, 269*f*

R

Reaction explorer, 191
Really Simple Syndication, 117, 118*f*
Reference management software, 58
Researchers behavior, changing patterns, 131
Resourcing chemical data online, 26
RSS. *See* Really Simple Syndication

S

Sceptical Chymists online, 95
Science
  bazaar, 107
  practice, 105
  teaching and learning, 106
Scientific literature and data access, 134
Semantically-enabled components
  SemanticEye, 45
  social Web-based scientific collaborations, 32
  Web 2.0, 44
  Web 3.0, 44
Semantic blogs, 54
SemanticEye
  group FOAF, 52*f*
  journal article, 47*f*
  personal FOAF, 51*f*
  SPARQL query, 50*f*, 51*f*
  triples, 51*f*
  XMP tool, 45, 47*f*
Semantic framework and ILE, 161, 161*t*
Semantic Web vocabulary
  FOAF, 48*f*
  social networks, 48
Situated learning, 170

Social bookmarking and student portal for learning, 297
Social networking
  chemical education, 7
  current status, 52
  learning, enhancing, 1
  Web 2.0 technologies, 56
Social tagging and information organization, 119
Social Web-based scientific collaborations
  resource, 44
  sciences, connecting, 32
  semantically-enabled components, 32
SPARQL
  FOAF aggregation, 49
  molecules of interest, identification, 50*f*
  queries, 49, 50, 50*f*, 51*f*
  scientist
    collaborators, identify, 50*f*
    same molecules, working, 50
  SemanticEye triples, 50*f*, 51*f*
Stoichiometry course, 238
Student assignments and wikipedia, 87
Student portal for learning
  assessment, 298
  daily pages and pathways, 295
  Diigo, 297
  lecture, 297
  meandering navigation, 296
  social bookmarking, 297
  student vs. teacher, 296
  textbook healthy, keep, 299
Symmetry Gallery, 74*f*

T

Textbook
  broken market, 271
  electronically, delivered, 285
    Bishop, Mark, 286
    ChemPaths, 287
    Connexions, 287
    DynamicBooks, 287
    eBooks, 286
    Learning to Meander, 287
    Wikibooks Web site, 286
  online, 283
    ChemPaths, 287
  page, screenshot, 292*f*
  student portal for learning, 295
17th Century foundation
  Royal Society, 100
  science education, tripartite nature, 97, 99
  social aspect, 99
Third millennium and bazaars, 106
Triplet relationship
  ChemPaths, 289
  osmotic pressure, image, 295*f*
  theoretical framework, 293
Twitter, 123

U

User knowledge state model, 200
University of Wisconsin–Madison students and cultural crossroads, 301*f*

V

Village people, 101
VIPEr. *See* Virtual Inorganic Pedagogical Electronic Resource
Virga on Mars and ChemPRIME exemplar, 270*f*
Virtual community of scientists, 95
Virtual Inorganic Pedagogical Electronic Resource
  homepage, 324*f*
  logo, 317*f*
  online teaching community, 312
Virtual laboratory
  collection, 237
  online practice questions, 247, 250*f*

W

Web 2.0
  blogs, 54
  Bob's virtual community of scientists, 95
  IONiC, 319*f*
  mashup, 57
  podcast, 56
  semantic blogs, 54
  Semantic Web technologies, 53
  social networks, 56
  technology changes, 97
  17th century foundation
    Royal Society, 100
    science, tripartite nature, 97
    science education, tripartite nature, 99
    social matters, 99
  wikis, 55
Web 3.0 and semantic enablement, 44

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Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ix002

Web background-history and e-Learning, 151
Web-based molecular visualization
  chemistry education, 65
  crystallography and inorganic chemistry, 75
  general chemistry, 70
  inorganic chemistry, 70
  interactivity
    adding, 68
    atomic orbitals, 69*f*
    3-D representations, 69*f*
    full, 69
  organic chemistry, 71
  viewing options, 68*f*
Web page and 3-D molecular models, 67
Weight scaling, 200
Wikibooks, 286
Wikipedia, 55, 81
  chemistry
    articles writing, 82
    content, 83, 84
    resource, 79, 80, 85
    student assignments, 87
  ChemPRIME, 263
  information presentation and synthesis, 122
  text, 263
Wordle tag cloud and online teaching community, 319*f*

X

Xanax, 33*f*, 34*f*

Y

Yakhchal in Kerman, Iran, 268*f*

Downloaded by 89.163.34.136 on June 23, 2012 | http://pubs.acs.org
Publication Date (Web): December 14, 2010 | doi: 10.1021/bk-2010-1060.ix002